Diphenylamine

Other names:	ANILINOBENZENE
	Aniline, N-phenyl-
	Benzenamine, N-phenyl-
	Benzene, (phenylamino)-
	Benzene, anilino-
	Big Dipper
	C.I. 10355
	DFA
	DPA
	Deccoscald 282
	Difenylamin
	N,N-Diphenylamine
	N-Fenylanilin
	N-PHENYL-BENZENAMINE
	N-Phenylaniline
	N-Phenylbenzenamine
	N-Phenylbenzeneamine
	NSC 215210
	Naugalube 428L
	No-Scald
	No-Scald dpa 283
	Phenylaniline
	Scaldip
Inchi:	InChI=1S/C12H11N/c1-3-7-11(8-4-1)13-12-9-5-2-6-10-12/h1-10,13H
InchiKey:	DMBHHRLKUKUOEG-UHFFFAOYSA-N
Formula:	C12H11N
SMILES:	c1ccc(Nc2ccccc2)cc1
Mol. weight [g/mol]:	169.22
CAS:	122-39-4

Physical Properties

Property code	Value	Unit	Source
chl	-6426.20	kJ/mol	NIST Webbook
gf	364.37	kJ/mol	Joback Method
hf	202.00	kJ/mol	NIST Webbook
hfl	132.00	kJ/mol	NIST Webbook

hfs	109.00	kJ/mol	NIST Webbook
hfs	131.00	kJ/mol	NIST Webbook
hfs	130.00 ± 1.50	kJ/mol	NIST Webbook
hfs	117.40 ± 2.10	kJ/mol	NIST Webbook
hfs	142.50	kJ/mol	NIST Webbook
hfus	19.68	kJ/mol	Measurement and prediction of (solid + liquid) equilibria of gun powder's and propellant's stabilizers mixtures
hsub	110.00	kJ/mol	NIST Webbook
hvap	70.00	kJ/mol	NIST Webbook
hvap	69.90	kJ/mol	NIST Webbook
hvap	55.23	kJ/mol	NIST Webbook
ie	7.19 ± 0.05	eV	NIST Webbook
ie	7.18 ± 0.01	eV	NIST Webbook
ie	7.14 ± 0.03	eV	NIST Webbook
ie	7.25 ± 0.03	eV	NIST Webbook
ie	7.44	eV	NIST Webbook
log10ws	-3.51		Aqueous Solubility Prediction Method
log10ws	-3.50		Estimated Solubility Method
logp	3.430		Crippen Method
mcvol	142.400	ml/mol	McGowan Method
nfpaf	%!d(float64=1)		KDB
nfpah	%!d(float64=3)		KDB
pc	8409.97 ± 405.30	kPa	NIST Webbook
rinpol	1601.00		NIST Webbook
rinpol	1617.00		NIST Webbook
rinpol	1568.00		NIST Webbook
rinpol	1575.00		NIST Webbook
rinpol	1637.00		NIST Webbook
rinpol	275.74		NIST Webbook
rinpol	1575.00		NIST Webbook
rinpol	1622.00		NIST Webbook
rinpol	1634.00		NIST Webbook
rinpol	274.57		NIST Webbook
rinpol	1602.00		NIST Webbook
rinpol	279.32		NIST Webbook
rinpol	276.00		NIST Webbook
rinpol	1619.00		NIST Webbook
rinpol	1567.00		NIST Webbook
rinpol	1621.00		NIST Webbook
rinpol	1625.00		NIST Webbook
rinpol	1637.00		NIST Webbook

rinpol	279.27		NIST Webbook
rinpol	1588.00		NIST Webbook
ripol	2521.00		NIST Webbook
ripol	2521.00		NIST Webbook
ripol	2517.00		NIST Webbook
ripol	2517.00		NIST Webbook
tb	575.15	K	KDB
tb	582.15 ± 2.00	K	NIST Webbook
tb	575.20	K	NIST Webbook
tc	931.15 ± 3.00	K	NIST Webbook
tf	325.60	K	Experimental and modeling studies of binary organic eutectic systems to be used as stabilizers for nitrate esters-based energetic materials
tf	325.85	K	KDB
tf	326.23	K	Aqueous Solubility Prediction Method
tf	326.65	K	DSC measurement and prediction of phase diagrams for binary mixtures of energetic materials' stabilizers
vc	0.526	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	404.16	J/mol×K	825.49	Joback Method
cpg	342.66	J/mol×K	618.82	Joback Method
cpg	357.24	J/mol×K	660.16	Joback Method
cpg	370.60	J/mol×K	701.49	Joback Method
cpg	382.81	J/mol×K	742.83	Joback Method
cpg	393.97	J/mol×K	784.16	Joback Method
cpg	326.77	J/mol×K	577.49	Joback Method
hfust	17.86	kJ/mol	326.20	NIST Webbook
hfust	17.86	kJ/mol	326.20	NIST Webbook
hfust	19.90	kJ/mol	326.10	NIST Webbook
hsubt	96.70 ± 2.50	kJ/mol	310.50	NIST Webbook
hsubt	110.00 ± 1.00	kJ/mol	311.00	NIST Webbook
hvapt	64.10	kJ/mol	478.00	NIST Webbook
hvapt	54.20	kJ/mol	623.00	NIST Webbook

psub	1.30e-04	kPa	302.10	Thermochemistry of Drugs. Experimental and First-Principles Study of Fenamates
psub	1.50e-04	kPa	302.70	Thermochemistry of Drugs. Experimental and First-Principles Study of Fenamates
psub	1.40e-04	kPa	303.20	Thermochemistry of Drugs. Experimental and First-Principles Study of Fenamates
psub	1.70e-04	kPa	305.20	Thermochemistry of Drugs. Experimental and First-Principles Study of Fenamates
psub	2.00e-04	kPa	305.50	Thermochemistry of Drugs. Experimental and First-Principles Study of Fenamates
psub	2.40e-04	kPa	308.00	Thermochemistry of Drugs. Experimental and First-Principles Study of Fenamates
psub	2.50e-04	kPa	308.00	Thermochemistry of Drugs. Experimental and First-Principles Study of Fenamates
psub	2.60e-04	kPa	308.20	Thermochemistry of Drugs. Experimental and First-Principles Study of Fenamates
psub	2.90e-04	kPa	309.10	Thermochemistry of Drugs. Experimental and First-Principles Study of Fenamates
psub	3.00e-04	kPa	309.30	Thermochemistry of Drugs. Experimental and First-Principles Study of Fenamates

psub	3.40e-04	kPa	310.70	Thermochemistry of Drugs. Experimental and First-Principles Study of Fenamates
psub	4.20e-04	kPa	312.30	Thermochemistry of Drugs. Experimental and First-Principles Study of Fenamates
psub	4.50e-04	kPa	313.00	Thermochemistry of Drugs. Experimental and First-Principles Study of Fenamates
psub	1.20e-04	kPa	301.00	Thermochemistry of Drugs. Experimental and First-Principles Study of Fenamates
psub	5.40e-04	kPa	315.00	Thermochemistry of Drugs. Experimental and First-Principles Study of Fenamates
psub	5.50e-04	kPa	315.00	Thermochemistry of Drugs. Experimental and First-Principles Study of Fenamates
psub	6.10e-04	kPa	315.40	Thermochemistry of Drugs. Experimental and First-Principles Study of Fenamates
psub	6.00e-04	kPa	315.70	Thermochemistry of Drugs. Experimental and First-Principles Study of Fenamates
psub	6.50e-04	kPa	316.00	Thermochemistry of Drugs. Experimental and First-Principles Study of Fenamates
psub	7.00e-04	kPa	316.70	Thermochemistry of Drugs. Experimental and First-Principles Study of Fenamates

psub	7.50e-04	kPa	317.20	Thermochemistry of Drugs. Experimental and First-Principles Study of Fenamates
psub	8.30e-04	kPa	318.00	Thermochemistry of Drugs. Experimental and First-Principles Study of Fenamates
psub	8.60e-04	kPa	318.20	Thermochemistry of Drugs. Experimental and First-Principles Study of Fenamates
psub	8.50e-04	kPa	318.30	Thermochemistry of Drugs. Experimental and First-Principles Study of Fenamates
psub	8.50e-04	kPa	318.70	Thermochemistry of Drugs. Experimental and First-Principles Study of Fenamates
psub	1.11e-03	kPa	320.30	Thermochemistry of Drugs. Experimental and First-Principles Study of Fenamates
psub	1.10e-03	kPa	320.70	Thermochemistry of Drugs. Experimental and First-Principles Study of Fenamates
psub	1.38e-03	kPa	322.30	Thermochemistry of Drugs. Experimental and First-Principles Study of Fenamates
psub	1.53e-03	kPa	323.20	Thermochemistry of Drugs. Experimental and First-Principles Study of Fenamates
psub	1.43e-03	kPa	323.20	Thermochemistry of Drugs. Experimental and First-Principles Study of Fenamates

psub	1.69e-03	kPa	324.10	Thermochemistry of Drugs. Experimental and First-Principles Study of Fenamates
psub	1.64e-03	kPa	324.70	Thermochemistry of Drugs. Experimental and First-Principles Study of Fenamates
psub	1.86e-03	kPa	325.20	Thermochemistry of Drugs. Experimental and First-Principles Study of Fenamates
psub	2.03e-03	kPa	326.70	Thermochemistry of Drugs. Experimental and First-Principles Study of Fenamates
psub	1.00e-04	kPa	300.20	Thermochemistry of Drugs. Experimental and First-Principles Study of Fenamates
psub	8.00e-05	kPa	298.40	Thermochemistry of Drugs. Experimental and First-Principles Study of Fenamates
psub	7.00e-05	kPa	298.20	Thermochemistry of Drugs. Experimental and First-Principles Study of Fenamates
psub	6.00e-05	kPa	296.20	Thermochemistry of Drugs. Experimental and First-Principles Study of Fenamates
psub	4.00e-05	kPa	293.70	Thermochemistry of Drugs. Experimental and First-Principles Study of Fenamates
psub	4.00e-05	kPa	293.10	Thermochemistry of Drugs. Experimental and First-Principles Study of Fenamates

psub	5.00e-04	kPa	313.70	Thermochemistry of Drugs. Experimental and First-Principles Study of Fenamates

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.53095e+01
Coeff. B	-5.43887e+03
Coeff. C	-6.64740e+01
Temperature range (K), min.	428.54
Temperature range (K), max.	610.47

Sources

Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C122394&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Experimental and modeling studies of binary organic eutectic systems to be used as stabilizers for nitrate esters based energetic materials:	https://www.doi.org/10.1016/j.fluid.2019.06.021
DSC measurement and prediction of phase diagrams for binary mixtures of energetic materials' stabilizers:	https://www.doi.org/10.1016/j.tca.2013.04.021
Thermochemistry of Drugs. Experimental and First-Principles Study of Fenamates:	https://www.doi.org/10.1021/je200128y
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Solubility of three natural compounds with insecticidal activity in supercritical carbon dioxide: Experimental measurements and predictive modeling with the GC-EoS:	https://www.doi.org/10.1016/j.fluid.2019.04.011
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Measurement and prediction of (solid + liquid) equilibria of gun powder's and propellant's stabilizers mixtures:	https://www.doi.org/10.1016/j.jct.2010.03.025
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1314.mol
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

Legend

chl:	Standard liquid enthalpy of combustion

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
nfpaf:	NFPA Fire Rating
nfpah:	NFPA Health Rating
pc:	Critical Pressure
psub:	Sublimation pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume