Naphthalene, 1-bromo-

Other names:	.alpha.-bromonaphthalene
	1-Bromonaphthalene
	1-Bromonapthalene
	1-NAPHTHYL BROMIDE
	ALPHA-BROMONAPHTHALENE
	«alpha»-Bromonaphthalene
	«alpha»-Naphthyl bromide
	Â«alphaÂ»-Bromonaphthalene
	Â«alphaÂ»-Naphthyl bromide
Inchi:	InChI=1S/C10H7Br/c11-10-7-3-5-8-4-1-2-6-9(8)10/h1-7H
InchiKey:	DLKQHBOKULLWDQ-UHFFFAOYSA-N
Formula:	C10H7Br
SMILES:	Brc1cccc2ccccc12
Mol. weight [g/mol]:	207.07
CAS:	90-11-9

Physical Properties

Property code	Value	Unit	Source
chl	-5024.90 ± 0.80	kJ/mol	NIST Webbook
chl	-5047.10 ± 2.20	kJ/mol	NIST Webbook
gf	257.07	kJ/mol	Joback Method
hf	174.30 ± 5.60	kJ/mol	NIST Webbook
hfl	111.60 ± 2.60	kJ/mol	NIST Webbook
hfus	17.61	kJ/mol	Joback Method
hvap	62.70 ± 5.00	kJ/mol	NIST Webbook
hvap	63.90 ± 0.40	kJ/mol	NIST Webbook
ie	8.08 ± 0.03	eV	NIST Webbook
ie	8.08 ± 0.03	eV	NIST Webbook
ie	8.09	eV	NIST Webbook
log10ws	-4.35		Estimated Solubility Method
log10ws	-4.35		Aqueous Solubility Prediction Method
logp	3.602		Crippen Method
mcvol	126.040	ml/mol	McGowan Method
pc	4173.09	kPa	Joback Method
rinpol	1434.00		NIST Webbook

rinpol	1434.00		NIST Webbook
rinpol	1434.00		NIST Webbook
ripol	2157.00		NIST Webbook
tb	554.25 ± 0.70	K	NIST Webbook
tb	554.20	K	NIST Webbook
tb	554.35	K	KDB
tc	800.62	K	Joback Method
tf	279.25 ± 0.30	K	NIST Webbook
tf	279.25 ± 0.20	K	NIST Webbook
tf	275.00 ± 1.00	K	NIST Webbook
tf	271.88	K	Aqueous Solubility Prediction Method
tf	279.25	K	KDB
vc	0.471	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	256.61	J/mol×K	587.60	Joback Method
cpg	267.49	J/mol×K	630.21	Joback Method
cpg	277.39	J/mol×K	672.81	Joback Method
cpg	302.26	J/mol×K	800.62	Joback Method
cpg	286.42	J/mol×K	715.42	Joback Method
cpg	294.68	J/mol×K	758.02	Joback Method
cpg	244.65	J/mol×K	545.00	Joback Method
dvisc	0.0004578	Pa×s	509.82	Joback Method
dvisc	0.0005467	Pa×s	474.63	Joback Method
dvisc	0.0006718	Pa×s	439.45	Joback Method
dvisc	0.0008557	Pa×s	404.27	Joback Method
dvisc	0.0011413	Pa×s	369.08	Joback Method
dvisc	0.0003922	Pa×s	545.00	Joback Method
dvisc	0.0016175	Pa×s	333.90	Joback Method
hfust	15.16	kJ/mol	271.40	NIST Webbook
hfust	15.16	kJ/mol	271.40	NIST Webbook
hvapt	56.00 ± 6.00	kJ/mol	327.00	NIST Webbook
hvapt	45.80	kJ/mol	514.00	NIST Webbook
hvapt	58.50	kJ/mol	456.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.90252e+01
Coeff. B	-6.39560e+03
Coeff. C	-6.65960e+01
Temperature range (K), min.	407.92
Temperature range (K), max.	532.96

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	9.46369e+01
Coeff. B	-1.12075e+04
Coeff. C	-1.12370e+01
Coeff. D	3.88225e-06
Temperature range (K), min.	279.35
Temperature range (K), max.	824.00

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Solubility of Bromoderivatives C60Brn (n = 6, 8, 24) in 1-Chloronaphthalene and 1-Bromonaphthalene in the Temperature Range (10 to 60) deg C: https://www.doi.org/10.1021/je100224a

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C90119&Units=SI

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

KDB: https://www.cheric.org/files/research/kdb/mol/mol1709.mol

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1709

Temperature Dependence of Solubility of Individual Light Fullerenes and Industrial Fullerene Mixture in 1-Chloronaphthalene and 1-Bromonaphthalene: https://www.doi.org/10.1021/je900814w

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion 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
pc:	Critical 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