Acridine

Other names:	10-Azaanthracene
	2,3-Benzoquinoline
	9-Azaanthracene
	Acrydine
	Akridin
	Benzo[b]quinoline
	Dibenzo[b,e]pyridine
	NSC 3408
	UN 2713
Inchi:	InChI=1S/C13H9N/c1-3-7-12-10(5-1)9-11-6-2-4-8-13(11)14-12/h1-9H
InchiKey:	DZBUGLKDJFMEHC-UHFFFAOYSA-N
Formula:	C13H9N
SMILES:	c1ccc2nc3ccccc3cc2c1
Mol. weight [g/mol]:	179.22
CAS:	260-94-6

Physical Properties

Property code	Value	Unit	Source
affp	972.60	kJ/mol	NIST Webbook
basg	940.70	kJ/mol	NIST Webbook
chs	-6602.80 ± 6.70	kJ/mol	NIST Webbook
chs	-6581.30 ± 0.90	kJ/mol	NIST Webbook
ea	0.90 ± 0.01	eV	NIST Webbook
ea	0.91 ± 0.10	eV	NIST Webbook
hf	273.90 ± 2.30	kJ/mol	NIST Webbook
hfs	179.40 ± 1.00	kJ/mol	NIST Webbook
hsub	92.80 ± 1.30	kJ/mol	NIST Webbook
hsub	90.80 ± 1.30	kJ/mol	NIST Webbook
hsub	94.50	kJ/mol	NIST Webbook
hsub	94.50	kJ/mol	NIST Webbook
hsub	94.50 ± 2.00	kJ/mol	NIST Webbook
hsub	93.30 ± 0.80	kJ/mol	NIST Webbook
hsub	91.70 ± 0.40	kJ/mol	NIST Webbook
ie	7.85	eV	NIST Webbook
ie	8.13 ± 0.02	eV	NIST Webbook
ie	7.80	eV	NIST Webbook
ie	8.04	eV	NIST Webbook

ie	8.00 ± 0.10	eV	NIST Webbook
ie	7.39	eV	NIST Webbook
ie	7.88 ± 0.02	eV	NIST Webbook
ie	7.80	eV	NIST Webbook
log10ws	-3.67		Estimated Solubility Method
log10ws	-3.67		Aqueous Solubility Prediction Method
logp	3.388		Crippen Method
mcvol	141.330	ml/mol	McGowan Method
rinpol	303.99		NIST Webbook
rinpol	1800.00		NIST Webbook
rinpol	1819.00		NIST Webbook
rinpol	1808.00		NIST Webbook
rinpol	1784.00		NIST Webbook
rinpol	1806.00		NIST Webbook
rinpol	1819.00		NIST Webbook
rinpol	303.30		NIST Webbook
rinpol	302.98		NIST Webbook
rinpol	303.18		NIST Webbook
rinpol	304.15		NIST Webbook
rinpol	304.04		NIST Webbook
rinpol	301.94		NIST Webbook
rinpol	304.50		NIST Webbook
rinpol	1819.00		NIST Webbook
rinpol	304.04		NIST Webbook
rinpol	308.10		NIST Webbook
rinpol	1806.00		NIST Webbook
rinpol	303.30		NIST Webbook
rinpol	301.94		NIST Webbook
rinpol	302.98		NIST Webbook
ss	208.00	J/mol×K	NIST Webbook
ss	208.03	J/mol×K	NIST Webbook
ss	208.03	J/mol×K	NIST Webbook
tb	618.70	K	NIST Webbook
tf	382.70 ± 5.00	K	NIST Webbook
tf	382.00 ± 5.00	K	NIST Webbook
tf	383.00 ± 5.00	K	NIST Webbook
tf	382.45 ± 1.00	K	NIST Webbook
tf	383.00 ± 3.00	K	NIST Webbook
tf	378.00 ± 6.00	K	NIST Webbook
tf	386.00 ± 3.00	K	NIST Webbook
tf	383.55 ± 0.30	K	NIST Webbook
tf	384.15 ± 1.50	K	NIST Webbook
tf	384.00 ± 2.00	K	NIST Webbook

tf	381.15 ± 3.00	K	NIST Webbook
tf	384.00 ± 3.00	K	NIST Webbook
tf	384.00 ± 3.00	K	NIST Webbook
tf	383.24	K	NIST Webbook
tf	381.65	K	Aqueous Solubility Prediction Method
tf	383.00 ± 5.00	K	NIST Webbook
tf	384.20 ± 0.20	K	NIST Webbook
tt	383.24 ± 0.01	K	NIST Webbook
tt	382.00	K	Thermodynamic study on six tricyclic nitrogen heterocyclic compounds by thermal analysis and effusion techniques

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	205.07	J/mol×K	298.15	NIST Webbook
cps	205.07	J/mol×K	298.15	NIST Webbook
cps	204.98	J/mol×K	298.15	NIST Webbook
hfust	20.68	kJ/mol	383.24	NIST Webbook
hfust	20.68	kJ/mol	383.24	NIST Webbook
hfust	18.58	kJ/mol	383.20	NIST Webbook
hfust	18.58	kJ/mol	383.20	NIST Webbook
hsubt	92.60	kJ/mol	304.00	NIST Webbook
hsubt	91.60 ± 2.50	kJ/mol	289.50	NIST Webbook
hsubt	92.00 ± 3.00	kJ/mol	281.20	NIST Webbook
hsubt	86.00	kJ/mol	430.00	NIST Webbook
hsubt	89.50 ± 0.20	kJ/mol	333.00	NIST Webbook
hvapt	61.50	kJ/mol	522.00	NIST Webbook
hvapt	62.90	kJ/mol	522.00	NIST Webbook
hvapt	62.10	kJ/mol	522.00	NIST Webbook
hvapt	71.50 ± 0.20	kJ/mol	510.00	NIST Webbook
hvapt	68.90 ± 0.10	kJ/mol	510.00	NIST Webbook
hvapt	66.40 ± 0.10	kJ/mol	510.00	NIST Webbook
hvapt	63.80 ± 0.10	kJ/mol	510.00	NIST Webbook
hvapt	61.30 ± 0.20	kJ/mol	510.00	NIST Webbook
hvapt	66.20	kJ/mol	510.50	NIST Webbook

rhos	1073.52	kg/m3	298.15	Liquid-Liquid Equilibria for Binary System of Ethanol + Hexadecane at Elevated Temperature and the Ternary Systems of Ethanol + Heterocyclic Nitrogen Compounds + Hexadecane at 298.15 K
sfust	53.97	J/mol×K	383.24	NIST Webbook
sfust	53.97	J/mol×K	383.24	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.53302e+01
Coeff. B	-6.03268e+03
Coeff. C	-5.55220e+01
Temperature range (K), min.	456.56
Temperature range (K), max.	657.66

Sources

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Experimental measurement and phase equilibria calculation for ternary systems of carbon dioxide+ toluene + naphthalene and carbon dioxide+ ethanol + acridine, applicable for fine particle production in GAS process:	https://www.doi.org/10.1016/j.tca.2016.06.007
Thermodynamic study on six tricyclic nitrogen heterocyclic compounds by thermal analysis and effusion techniques:	https://www.doi.org/10.1016/j.tca.2016.05.001
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C260946&Units=SI
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Liquid-Liquid Equilibria for Binary System of Ethanol + Hexadecane at Elevated Temperature and the Ternary Systems of Ethanol + Heterocyclic Nitrogen Compounds + Hexadecane at 298.15 K:	https://www.doi.org/10.1021/je700233p
Infinite Dilution Binary Diffusion Coefficients of Hydrotreating Compounds in Tetradecane in the Temperature Range from (310 to 475) K:	https://www.doi.org/10.1021/je700535q
Thermodynamic properties of three-ring azaaromatics. 1. Experimental results for phenazine and acridine, and mutual validation of experiments and computational methods:	https://www.doi.org/10.1016/j.jct.2009.11.010
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Legend

affp:	Proton affinity
basg:	Gas basicity
chs:	Standard solid enthalpy of combustion
cps:	Solid phase heat capacity
ea:	Electron affinity
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation 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
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
pvap:	Vapor pressure
rhos:	Solid Density
rinpol:	Non-polar retention indices
sfust:	Entropy of fusion at a given temperature
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature