6-Chrysenamine

Other names:	6-Amc
	6-Aminochrysene
	Chrysenex
	Chrysonex
	chrysen-6-ylamine
Inchi:	InChI=1S/C18H13N/c19-18-11-17-13-6-2-1-5-12(13)9-10-15(17)14-7-3-4-8-16(14)18/h1-
InchiKey:	KIVUHCNVDWYUNP-UHFFFAOYSA-N
Formula:	C18H13N
SMILES:	Nc1cc2c3ccccc3ccc2c2ccccc12
Mol. weight [g/mol]:	243.30
CAS:	2642-98-0

Physical Properties

Property code	Value	Unit	Source
gf	570.60	kJ/mol	Joback Method
hf	394.27	kJ/mol	Joback Method
hfus	31.50	kJ/mol	Joback Method
hvap	75.48	kJ/mol	Joback Method
ie	7.00 ± 0.10	eV	NIST Webbook
log10ws	-6.20		Aqueous Solubility Prediction Method
log10ws	-6.20		Estimated Solubility Method
logp	4.728		Crippen Method
mcvol	192.320	ml/mol	McGowan Method
pc	2865.80	kPa	Joback Method
rinpol	463.19		NIST Webbook
rinpol	452.52		NIST Webbook
tb	782.33	K	Joback Method
tc	1050.06	K	Joback Method
tf	483.65	K	Aqueous Solubility Prediction Method
vc	0.731	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	523.87	J/mol×K	782.33	Joback Method
cpg	537.53	J/mol×K	826.95	Joback Method
cpg	550.29	J/mol×K	871.57	Joback Method
cpg	562.36	J/mol×K	916.19	Joback Method
cpg	573.96	J/mol×K	960.81	Joback Method
cpg	585.32	J/mol×K	1005.44	Joback Method
cpg	596.64	J/mol×K	1050.06	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2642980&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method: https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Legend

cpg: Ideal gas heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point

vc: Critical Volume