Acridine, 9,10-dihydro-

Other names:	Acridan
	Acridane
	Carbazine
	9,10-Dihydroacridine
Inchi:	InChI=1S/C13H11N/c1-3-7-12-10(5-1)9-11-6-2-4-8-13(11)14-12/h1-8,14H,9H2
InchiKey:	HJCUTNIGJHJGCF-UHFFFAOYSA-N
Formula:	C13H11N
SMILES:	c1ccc2c(c1)Cc1ccccc1N2
Mol. weight [g/mol]:	181.23
CAS:	92-81-9

Physical Properties

Property code	Value	Unit	Source
gf	432.41	kJ/mol	Joback Method
hf	275.58	kJ/mol	Joback Method
hfus	25.48	kJ/mol	Joback Method
hvap	57.22	kJ/mol	Joback Method
ie	7.33	eV	NIST Webbook
ie	7.24 ± 0.03	eV	NIST Webbook
log10ws	-3.62		Crippen Method
logp	3.334		Crippen Method
mcvol	145.630	ml/mol	McGowan Method
pc	3581.35	kPa	Joback Method
rinpol	304.11		NIST Webbook
rinpol	279.00		NIST Webbook
rinpol	304.33		NIST Webbook
tb	615.85	K	Joback Method
tc	875.48	K	Joback Method
tf	444.88	K	Joback Method
vc	0.550	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	348.81	J/mol×K	615.85	Joback Method
cpg	363.98	J/mol×K	659.12	Joback Method
cpg	377.88	J/mol×K	702.39	Joback Method
cpg	390.64	J/mol×K	745.67	Joback Method
cpg	402.38	J/mol×K	788.94	Joback Method
cpg	413.24	J/mol×K	832.21	Joback Method
cpg	423.34	J/mol×K	875.48	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C92819&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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