2-(1-Methylethyl)perimidine

Other names: 2-Isopropyl-1H-perimidine
Inchi: InChI=1S/C14H14N2/c1-9(2)14-15-11-7-3-5-10-6-4-8-12(16-14)13(10)11/h3-9H,1-2H3,(H
InchiKey: RYNTXOSYMIOQJA-UHFFFAOYSA-N
Formula: C14H14N2
SMILES: CC(C)C1=Nc2cccc3cccc(c23)N1
Mol. weight [g/mol]: 210.27
CAS: 28478-14-0

Physical Properties

Property code	Value	Unit	Source
gf	557.64	kJ/mol	Joback Method
hf	315.32	kJ/mol	Joback Method
hfus	31.40	kJ/mol	Joback Method
hvap	65.75	kJ/mol	Joback Method
log10ws	-4.42		Crippen Method
logp	3.951		Crippen Method
mcvol	169.700	ml/mol	McGowan Method
pc	3093.29	kPa	Joback Method
rinpol	2047.00		NIST Webbook
tb	692.70	K	Joback Method
tc	949.73	K	Joback Method
tf	528.73	K	Joback Method
vc	0.657	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	460.72	J/mol×K	692.70	Joback Method
cpg	476.63	J/mol×K	735.54	Joback Method
cpg	491.30	J/mol×K	778.38	Joback Method
cpg	504.83	J/mol×K	821.21	Joback Method
cpg	517.32	J/mol×K	864.05	Joback Method
cpg	528.89	J/mol×K	906.89	Joback Method
cpg	539.64	J/mol×K	949.73	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=C28478140&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
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