Acenaphthylene-1-carbonitrile

Inchi: InChI=1S/C13H7N/c14-8-11-7-10-5-1-3-9-4-2-6-12(11)13(9)10/h1-7H
InchiKey: SGMUADOXMCAHTK-UHFFFAOYSA-N
Formula: C13H7N
SMILES: N#CC1=Cc2cccc3cccc1c23
Mol. weight [g/mol]: 177.20

Physical Properties

Property code	Value	Unit	Source
gf	492.45	kJ/mol	Joback Method
hf	403.50	kJ/mol	Joback Method
hfus	21.21	kJ/mol	Joback Method
hvap	61.25	kJ/mol	Joback Method
log10ws	-4.41		Crippen Method
logp	3.217		Crippen Method
mcvol	137.030	ml/mol	McGowan Method
pc	3135.00	kPa	Joback Method
rinpol	302.00		NIST Webbook
tb	665.82	K	Joback Method
tc	919.15	K	Joback Method
tf	424.40	K	Joback Method
vc	0.555	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	323.13	J/mol×K	665.82	Joback Method
cpg	333.10	J/mol×K	708.04	Joback Method
cpg	342.26	J/mol×K	750.26	Joback Method
cpg	350.77	J/mol×K	792.48	Joback Method
cpg	358.78	J/mol×K	834.70	Joback Method
cpg	366.42	J/mol×K	876.92	Joback Method
cpg	373.86	J/mol×K	919.15	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R312577&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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