1-Cyano-2-ethyl-naphthalene

Inchi: InChI=1S/C13H11N/c1-2-10-7-8-11-5-3-4-6-12(11)13(10)9-14/h3-8H,2H2,1H3
InchiKey: AFBHQTVEDHVZTB-UHFFFAOYSA-N
Formula: C13H11N
SMILES: CCc1ccc2ccccc2c1C#N
Mol. weight [g/mol]: 181.23
CAS: 103408-11-3

Physical Properties

Property code	Value	Unit	Source
gf	391.56	kJ/mol	Joback Method
hf	257.89	kJ/mol	Joback Method
hfus	21.21	kJ/mol	Joback Method
hvap	60.25	kJ/mol	Joback Method
log10ws	-4.43		Crippen Method
logp	3.274		Crippen Method
mcvol	152.190	ml/mol	McGowan Method
pc	2643.39	kPa	Joback Method
tb	654.54	K	Joback Method
tc	895.82	K	Joback Method
tf	385.42	K	Joback Method
vc	0.604	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	367.95	J/mol×K	654.54	Joback Method
cpg	380.46	J/mol×K	694.75	Joback Method
cpg	392.05	J/mol×K	734.97	Joback Method
cpg	402.81	J/mol×K	775.18	Joback Method
cpg	412.81	J/mol×K	815.39	Joback Method
cpg	422.13	J/mol×K	855.60	Joback Method
cpg	430.84	J/mol×K	895.82	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C103408113&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume