1-Cyano-4-methylnaphthalene

Inchi: InChI=1S/C12H9N/c1-9-6-7-10(8-13)12-5-3-2-4-11(9)12/h2-7H,1H3
InchiKey: XDIWTJZAYBYKHM-UHFFFAOYSA-N
Formula: C12H9N
SMILES: Cc1ccc(C#N)c2ccccc12
Mol. weight [g/mol]: 167.21
CAS: 36062-93-8

Physical Properties

Property code	Value	Unit	Source
gf	383.14	kJ/mol	Joback Method
hf	278.53	kJ/mol	Joback Method
hfus	18.62	kJ/mol	Joback Method
hvap	58.02	kJ/mol	Joback Method
log10ws	-4.10		Crippen Method
logp	3.020		Crippen Method
mcvol	138.100	ml/mol	McGowan Method
pc	2925.00	kPa	Joback Method
tb	631.66	K	Joback Method
tc	878.27	K	Joback Method
tf	374.15	K	Joback Method
vc	0.547	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	320.00	J/mol×K	631.66	Joback Method
cpg	331.73	J/mol×K	672.76	Joback Method
cpg	342.56	J/mol×K	713.86	Joback Method
cpg	352.58	J/mol×K	754.96	Joback Method
cpg	361.85	J/mol×K	796.06	Joback Method
cpg	370.46	J/mol×K	837.17	Joback Method
cpg	378.48	J/mol×K	878.27	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=C36062938&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume