2-[1-(4-Cyano-1,2,3,4-tetrahydronaphthyl)]propan

Other names: 4-(1-Cyanoethyl)-1,2,3,4-tetrahydro-1-naphthalenecarbonitrile
Inchi: InChI=1S/C14H14N2/c1-10(8-15)12-7-6-11(9-16)13-4-2-3-5-14(12)13/h2-5,10-12H,6-7H2
InchiKey: FDTQTOKRWQJRAC-UHFFFAOYSA-N
Formula: C14H14N2
SMILES: CC(C#N)C1CCC(C#N)c2ccccc21
Mol. weight [g/mol]: 210.27
CAS: 57964-39-3

Physical Properties

Property code	Value	Unit	Source
gf	474.64	kJ/mol	Joback Method
hf	263.55	kJ/mol	Joback Method
hfus	22.26	kJ/mol	Joback Method
hvap	70.04	kJ/mol	Joback Method
log10ws	-4.07		Crippen Method
logp	3.331		Crippen Method
mcvol	176.260	ml/mol	McGowan Method
pc	2131.49	kPa	Joback Method
rinpol	2078.00		NIST Webbook
rinpol	2078.00		NIST Webbook
rinpol	2078.00		NIST Webbook
tb	761.44	K	Joback Method
tc	1007.47	K	Joback Method
tf	411.64	K	Joback Method
vc	0.706	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	496.03	J/mol×K	761.44	Joback Method
cpg	509.67	J/mol×K	802.44	Joback Method
cpg	522.23	J/mol×K	843.45	Joback Method
cpg	533.80	J/mol×K	884.45	Joback Method
cpg	544.45	J/mol×K	925.46	Joback Method

cpg	554.26	J/mol×K	966.46	Joback Method
cpg	563.30	J/mol×K	1007.47	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C57964393&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume