1-Norbornylisocyanide

Inchi: InChI=1S/C8H11N/c1-9-8-4-2-7(6-8)3-5-8/h7H,2-6H2
InchiKey: ZGHGUYUIGKWVIH-UHFFFAOYSA-N
Formula: C8H11N
SMILES: [C-]#[N+]C12CCC(CC1)C2
Mol. weight [g/mol]: 121.18
CAS: 103434-09-9

Physical Properties

Property code	Value	Unit	Source
chs	-4825.40 ± 4.60	kJ/mol	NIST Webbook
gf	253.57	kJ/mol	Joback Method
hf	165.80 ± 4.60	kJ/mol	NIST Webbook
hfs	105.20 ± 4.60	kJ/mol	NIST Webbook
hfus	5.85	kJ/mol	Joback Method
hsub	60.60	kJ/mol	NIST Webbook
hsub	60.58 ± 0.50	kJ/mol	NIST Webbook
hsub	60.60 ± 0.50	kJ/mol	NIST Webbook
hvap	42.73	kJ/mol	Joback Method
log10ws	-4.60		Crippen Method
logp	2.238		Crippen Method
mcvol	103.240	ml/mol	McGowan Method
pc	3538.87	kPa	Joback Method
tb	502.51	K	Joback Method
tc	736.30	K	Joback Method
tf	301.17	K	Joback Method
vc	0.413	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	300.53	J/mol×K	697.33	Joback Method
cpg	240.63	J/mol×K	502.51	Joback Method
cpg	254.79	J/mol×K	541.47	Joback Method
cpg	267.67	J/mol×K	580.44	Joback Method

cpg	279.46	J/mol×K	619.40	Joback Method
cpg	290.35	J/mol×K	658.37	Joback Method
cpg	310.21	J/mol×K	736.30	Joback Method
cps	196.70	J/mol×K	298.15	NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C103434099&Units=SI

Legend

chs: Standard solid enthalpy of combustion
cpg: Ideal gas heat capacity
cps: Solid phase heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfs: Solid phase enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hsub: Enthalpy of sublimation 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