

1-Norbornyl cyanide

Inchi:

lnchl=1S/C8H11N/c9-6-8-3-1-7(5-8)2-4-8/h7H,1-5H2

InchiKey:

OJDABTNGJHBQFD-UHFFFAOYSA-N

Formula:

C8H11N

SMILES:

N#CC12CCC(CC1)C2

Mol. weight [g/mol]:

121.18

CAS:

88523-51-7

Physical Properties

Property code	Value	Unit	Source
chs	-4733.40 ± 1.30	kJ/mol	NIST Webbook
gf	253.57	kJ/mol	Joback Method
hf	75.20 ± 2.00	kJ/mol	NIST Webbook
hfs	13.30 ± 1.30	kJ/mol	NIST Webbook
hfus	5.85	kJ/mol	Joback Method
hsub	61.90	kJ/mol	NIST Webbook
hsub	61.90 ± 1.50	kJ/mol	NIST Webbook
hvap	42.73	kJ/mol	Joback Method
log10ws	-2.34		Crippen Method
logp	2.090		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	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	300.53	J/mol×K	697.33	Joback Method
cpg	310.21	J/mol×K	736.30	Joback Method
cps	172.90	J/mol×K	298.15	NIST Webbook

Sources

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=C88523517&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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