Diisopropylcyanamide

Other names:	Cyanamide, bis(1-methylethyl)-
	Cyanamide, diisopropyl-
	Diisopropylcyanimide
Inchi:	InChI=1S/C7H14N2/c1-6(2)9(5-8)7(3)4/h6-7H,1-4H3
InchiKey:	DGCUISYKMONQDH-UHFFFAOYSA-N
Formula:	C7H14N2
SMILES:	CC(C)N(C#N)C(C)C
Mol. weight [g/mol]:	126.20
CAS:	3085-76-5

Physical Properties

Property code	Value	Unit	Source
chl	-4704.03	kJ/mol	NIST Webbook
gf	247.14	kJ/mol	Joback Method
hf	34.04	kJ/mol	Joback Method
hfl	-51.42	kJ/mol	NIST Webbook
hfus	11.37	kJ/mol	Joback Method
hvap	42.92	kJ/mol	Joback Method
log10ws	-1.91		Crippen Method
logp	1.586		Crippen Method
mcvol	120.850	ml/mol	McGowan Method
pc	2767.17	kPa	Joback Method
tb	473.20	K	Joback Method
tc	666.47	K	Joback Method
tf	244.84 ± 0.60	K	NIST Webbook
tf	245.85 ± 0.30	K	NIST Webbook
vc	0.460	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	260.53	J/mol×K	473.20	Joback Method
cpg	272.68	J/mol×K	505.41	Joback Method
cpg	284.24	J/mol×K	537.62	Joback Method

cpg	295.21	J/mol×K	569.84	Joback Method
cpg	305.62	J/mol×K	602.05	Joback Method
cpg	315.49	J/mol×K	634.26	Joback Method
cpg	324.84	J/mol×K	666.47	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	366.70	K	3.30	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=C3085765&Units=SI

Legend

chl: Standard liquid enthalpy of combustion
cpg: Ideal gas heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfl: Liquid phase 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
tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point

vc: Critical Volume