1,1-Dicyanoethane

Other names: Malononitrile, methyl-
Propanedinitrile, methyl-
Methylmalononitrile
Methyl-malonitril
Methylpropanedinitrile
Inchi: InChI=1S/C4H4N2/c1-4(2-5)3-6/h4H,1H3
InchiKey: LXUTYOVUICAOGH-UHFFFAOYSA-N
Formula: C4H4N2
SMILES: CC(C#N)C#N
Mol. weight [g/mol]: 80.09
CAS: 3696-36-4

Physical Properties

Property code	Value	Unit	Source
gf	246.72	kJ/mol	Joback Method
hf	198.59	kJ/mol	Joback Method
hfus	5.61	kJ/mol	Joback Method
hvap	45.07	kJ/mol	Joback Method
log10ws	-0.99		Crippen Method
logp	0.670		Crippen Method
mcvol	69.980	ml/mol	McGowan Method
pc	3699.95	kPa	Joback Method
tb	494.64	K	Joback Method
tc	714.45	K	Joback Method
tf	249.82	K	Joback Method
vc	0.305	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	129.63	J/mol×K	494.64	Joback Method
cpg	134.73	J/mol×K	531.27	Joback Method
cpg	139.57	J/mol×K	567.91	Joback Method
cpg	144.15	J/mol×K	604.54	Joback Method

cpg	148.48	J/mol×K	641.18	Joback Method
cpg	152.57	J/mol×K	677.81	Joback Method
cpg	156.43	J/mol×K	714.45	Joback Method

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=C3696364&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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