Propanedinitrile, dimethyl-

Other names:	Malononitrile, dimethyl- Dimethylmalononitrile 2,2-Dicyanopropane
Inchi:	InChI=1S/C5H6N2/c1-5(2,3-6)4-7/h1-2H3
InchiKey:	BCMJJXWXMZYZKN-UHFFFAOYSA-N
Formula:	C5H6N2
SMILES:	CC(C)(C#N)C#N
Mol. weight [g/mol]:	94.11
CAS:	7321-55-3

Physical Properties

Property code	Value	Unit	Source
chs	-2960.20 ± 0.71	kJ/mol	NIST Webbook
gf	260.42	kJ/mol	Joback Method
hf	197.20 ± 1.00	kJ/mol	NIST Webbook
hfs	135.20 ± 0.20	kJ/mol	NIST Webbook
hfus	4.30	kJ/mol	Joback Method
hsub	61.97 ± 0.71	kJ/mol	NIST Webbook
hsub	62.00	kJ/mol	NIST Webbook
hsub	62.00 ± 0.70	kJ/mol	NIST Webbook
hvap	46.38	kJ/mol	Joback Method
ie	12.39	eV	NIST Webbook
log10ws	-1.41		Crippen Method
logp	1.060		Crippen Method
mcvol	84.070	ml/mol	McGowan Method
pc	3345.11	kPa	Joback Method
tb	442.70	K	NIST Webbook
tc	740.17	K	Joback Method
tf	278.51	K	Joback Method
tt	307.47 ± 0.02	K	NIST Webbook
vc	0.356	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	206.39	J/mol×K	740.17	Joback Method
cpg	178.72	J/mol×K	552.30	Joback Method
cpg	185.13	J/mol×K	589.88	Joback Method
cpg	191.07	J/mol×K	627.45	Joback Method
cpg	196.57	J/mol×K	665.02	Joback Method
cpg	201.66	J/mol×K	702.59	Joback Method
cpg	171.80	J/mol×K	514.73	Joback Method
hfust	4.05	kJ/mol	307.50	NIST Webbook
hfust	9.87	kJ/mol	302.60	NIST Webbook
hfust	4.05	kJ/mol	307.50	NIST Webbook
hvapt	47.50	kJ/mol	367.50	NIST Webbook
sfust	32.59	J/mol×K	302.60	NIST Webbook
sfust	13.18	J/mol×K	307.50	NIST Webbook

Sources

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=C7321553&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chs: Standard solid enthalpy of combustion
cpg: Ideal gas 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
hfust: Enthalpy of fusion at a given temperature
hsub: Enthalpy of sublimation at standard conditions
hvap: Enthalpy of vaporization at standard conditions
hvapt: Enthalpy of vaporization at a given temperature
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient

mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume