Methyl(1,1,2-trimethylpropyl)malononitrile

Inchi: InChI=1S/C10H16N2/c1-8(2)9(3,4)10(5,6-11)7-12/h8H,1-5H3
InchiKey: ZMCKYPPOTHYZAA-UHFFFAOYSA-N
Formula: C10H16N2
SMILES: CC(C)C(C)(C)C(C)(C#N)C#N
Mol. weight [g/mol]: 164.25
CAS: 85688-96-6

Physical Properties

Property code	Value	Unit	Source
chs	-6239.01 ± 0.63	kJ/mol	NIST Webbook
gf	302.92	kJ/mol	Joback Method
hf	79.33 ± 0.96	kJ/mol	NIST Webbook
hfs	17.30 ± 0.63	kJ/mol	NIST Webbook
hfus	6.32	kJ/mol	Joback Method
hsub	62.00	kJ/mol	NIST Webbook
hsub	62.00 ± 0.70	kJ/mol	NIST Webbook
hsub	62.05 ± 0.71	kJ/mol	NIST Webbook
hvap	55.83	kJ/mol	Joback Method
log10ws	-3.02		Crippen Method
logp	2.722		Crippen Method
mcvol	154.520	ml/mol	McGowan Method
pc	2100.34	kPa	Joback Method
tb	625.46	K	Joback Method
tc	848.98	K	Joback Method
tf	322.28	K	Joback Method
vc	0.620	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	396.73	J/mol×K	625.46	Joback Method
cpg	409.43	J/mol×K	662.71	Joback Method
cpg	421.22	J/mol×K	699.97	Joback Method
cpg	432.15	J/mol×K	737.22	Joback Method

cpg	442.32	J/mol×K	774.47	Joback Method
cpg	451.79	J/mol×K	811.73	Joback Method
cpg	460.64	J/mol×K	848.98	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C85688966&Units=SI
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

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
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