4,4-Dimethyl-3-oxopentanenitrile

Other names:	Pivaloylacetonitrile
	Trimethylacetylacetonitrile
	Pentanenitrile, 4,4-dimethyl-3-oxo-
	4,4-dimethyl-3-oxovaleronitrile
Inchi:	InChI=1S/C7H11NO/c1-7(2,3)6(9)4-5-8/h4H2,1-3H3
InchiKey:	MXZMACXOMZKYHJ-UHFFFAOYSA-N
Formula:	C7H11NO
SMILES:	CC(C)(C)C(=O)CC#N
Mol. weight [g/mol]:	125.17
CAS:	59997-51-2

Physical Properties

Property code	Value	Unit	Source
gf	15.16	kJ/mol	Joback Method
hf	-144.26	kJ/mol	Joback Method
hfus	9.58	kJ/mol	Joback Method
hvap	47.10	kJ/mol	Joback Method
log10ws	-1.66		Crippen Method
logp	1.515		Crippen Method
mcvol	112.440	ml/mol	McGowan Method
pc	2976.29	kPa	Joback Method
tb	512.28	K	Joback Method
tc	721.65	K	Joback Method
tf	285.99	K	Joback Method
vc	0.449	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	247.32	J/mol×K	512.28	Joback Method
cpg	257.87	J/mol×K	547.17	Joback Method
cpg	267.76	J/mol×K	582.07	Joback Method
cpg	277.03	J/mol×K	616.96	Joback Method
cpg	285.72	J/mol×K	651.86	Joback Method

cpg	293.85	J/mol×K	686.75	Joback Method
cpg	301.47	J/mol×K	721.65	Joback Method

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=C59997512&Units=SI

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