Propanedinitrile, (acetyloxy)methyl-

Other names:	Tartrononitrile, methyl-, acetate (ester)
	«alpha»,«alpha»-Dicyanoethyl acetate
	Malononitrile, hydroxymethyl-, acetate (ester)
	1-Acetoxxy-1,1-dicyanoethane
	1-Acetoxy-1,1-dicyanoethane
	1,1-Dicyanoethyl acetate
	2-Acetoxyisosuccinodinitrile
	Tartrononitrile, methyl-, acetate
	Acetic acid 1,1-dicyanoethyl ester
	1,1-Dikyanethylester kyseliny octove
	Methylacetoxymalonitrile
	Methylacetoxymalononitrile
	NSC 6394
	Propanedinitrile, 2-(acetyloxy)-2-methyl-
Inchi:	InChI=1S/C6H6N2O2/c1-5(9)10-6(2,3-7)4-8/h1-2H3
InchiKey:	OSNAAKXQIFQLNS-UHFFFAOYSA-N
Formula:	C6H6N2O2
SMILES:	CC(=O)OC(C)(C#N)C#N
Mol. weight [g/mol]:	138.12
CAS:	7790-01-4

Physical Properties

Property code	Value	Unit	Source
gf	34.92	kJ/mol	Joback Method
hf	-90.96	kJ/mol	Joback Method
hfus	9.68	kJ/mol	Joback Method
hvap	57.77	kJ/mol	Joback Method
log10ws	-1.04		Crippen Method
logp	0.355		Crippen Method
mcvol	105.600	ml/mol	McGowan Method
pc	3159.72	kPa	Joback Method
tb	613.90	K	Joback Method
tc	840.26	K	Joback Method
tf	361.94	K	Joback Method
vc	0.436	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	239.62	J/mol×K	613.90	Joback Method
cpg	246.69	J/mol×K	651.63	Joback Method
cpg	253.25	J/mol×K	689.35	Joback Method
cpg	259.34	J/mol×K	727.08	Joback Method
cpg	264.97	J/mol×K	764.81	Joback Method
cpg	270.16	J/mol×K	802.54	Joback Method
cpg	274.92	J/mol×K	840.26	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7790014&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

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