

Propanoic acid, 3-cyano-, methyl ester

Other names:	Propionic acid, 3-cyano-, methyl ester Methyl «beta»-cyanopropionate Methyl 3-cyanopropionate 3-Cyanopropionic acid, methyl ester Methyl cyanopropanoate Methyl 3-cyanopropanoate
Inchi:	InChI=1S/C5H7NO2/c1-8-5(7)3-2-4-6/h2-3H2,1H3
InchiKey:	BPSKURPOKFSLHJ-UHFFFAOYSA-N
Formula:	C5H7NO2
SMILES:	COC(=O)CCC#N
Mol. weight [g/mol]:	113.11
CAS:	4107-62-4

Physical Properties

Property code	Value	Unit	Source
gf	-109.52	kJ/mol	Joback Method
hf	-226.45	kJ/mol	Joback Method
hfus	13.00	kJ/mol	Joback Method
hvap	46.36	kJ/mol	Joback Method
log10ws	-0.64		Crippen Method
logp	0.463		Crippen Method
mcvol	90.130	ml/mol	McGowan Method
pc	3555.77	kPa	Joback Method
tb	492.17	K	Joback Method
tc	692.81	K	Joback Method
tf	283.26	K	Joback Method
vc	0.365	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	183.09	J/mol×K	492.17	Joback Method
cpg	190.32	J/mol×K	525.61	Joback Method
cpg	197.29	J/mol×K	559.05	Joback Method

cpg	203.97	J/mol×K	592.49	Joback Method
cpg	210.38	J/mol×K	625.93	Joback Method
cpg	216.49	J/mol×K	659.37	Joback Method
cpg	222.32	J/mol×K	692.81	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4107624&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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