3,3,3-Trimethoxypropionitrile

Inchi: InChI=1S/C6H11NO3/c1-8-6(9-2,10-3)4-5-7/h4H2,1-3H3
InchiKey: IPJDXQYLAATRJK-UHFFFAOYSA-N
Formula: C6H11NO3
SMILES: COC(CC#N)(OC)OC
Mol. weight [g/mol]: 145.16
CAS: 70138-31-7

Physical Properties

Property code	Value	Unit	Source
gf	-179.34	kJ/mol	Joback Method
hf	-407.70	kJ/mol	Joback Method
hfus	8.95	kJ/mol	Joback Method
hvap	55.90 ± 4.20	kJ/mol	NIST Webbook
log10ws	-0.56		Crippen Method
logp	0.493		Crippen Method
mcvol	114.390	ml/mol	McGowan Method
pc	2918.68	kPa	Joback Method
tb	502.79	K	Joback Method
tc	700.43	K	Joback Method
tf	291.48	K	Joback Method
vc	0.441	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	257.32	J/mol×K	502.79	Joback Method
cpg	267.17	J/mol×K	535.73	Joback Method
cpg	276.64	J/mol×K	568.67	Joback Method
cpg	285.73	J/mol×K	601.61	Joback Method
cpg	294.43	J/mol×K	634.55	Joback Method
cpg	302.73	J/mol×K	667.49	Joback Method
cpg	310.63	J/mol×K	700.43	Joback Method

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=C70138317&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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