Acetic acid, cyano-, 2-methoxyethyl ester

Other names: 2-Methoxyethyl cyanoacetate
Inchi: InChI=1S/C6H9NO3/c1-9-4-5-10-6(8)2-3-7/h2,4-5H2,1H3
InchiKey: SGLKIEOMYXTGBH-UHFFFAOYSA-N
Formula: C6H9NO3
SMILES: COCCOC(=O)CC#N
Mol. weight [g/mol]: 143.14
CAS: 10258-54-5

Physical Properties

Property code	Value	Unit	Source
gf	-206.10	kJ/mol	Joback Method
hf	-379.31	kJ/mol	Joback Method
hfus	16.78	kJ/mol	Joback Method
hvap	50.99	kJ/mol	Joback Method
log10ws	-0.15		Crippen Method
logp	0.090		Crippen Method
mcvol	110.090	ml/mol	McGowan Method
pc	3121.00	kPa	Joback Method
tb	537.47	K	Joback Method
tc	733.83	K	Joback Method
tf	316.76	K	Joback Method
vc	0.440	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	244.20	J/mol×K	537.47	Joback Method
cpg	252.72	J/mol×K	570.20	Joback Method
cpg	260.94	J/mol×K	602.92	Joback Method
cpg	268.84	J/mol×K	635.65	Joback Method
cpg	276.41	J/mol×K	668.38	Joback Method
cpg	283.64	J/mol×K	701.10	Joback Method
cpg	290.51	J/mol×K	733.83	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=C10258545&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