n-Propyl cyanoacetate

Other names: Acetic acid, cyano-, propyl ester
propyl cyanoacetate
Inchi: InChI=1S/C6H9NO2/c1-2-5-9-6(8)3-4-7/h2-3,5H2,1H3
InchiKey: NLFIMXLLXGTDME-UHFFFAOYSA-N
Formula: C6H9NO2
SMILES: CCCOC(=O)CC#N
Mol. weight [g/mol]: 127.14
CAS: 14447-15-5

Physical Properties

Property code	Value	Unit	Source
gf	-101.10	kJ/mol	Joback Method
hf	-247.09	kJ/mol	Joback Method
hfus	15.59	kJ/mol	Joback Method
hvap	48.58	kJ/mol	Joback Method
log10ws	-1.06		Crippen Method
logp	0.853		Crippen Method
mcvol	104.220	ml/mol	McGowan Method
pc	3181.14	kPa	Joback Method
tb	515.05	K	Joback Method
tc	713.00	K	Joback Method
tf	294.53	K	Joback Method
vc	0.421	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	223.28	J/mol×K	515.05	Joback Method
cpg	231.80	J/mol×K	548.04	Joback Method
cpg	239.97	J/mol×K	581.03	Joback Method
cpg	247.80	J/mol×K	614.02	Joback Method
cpg	255.27	J/mol×K	647.01	Joback Method
cpg	262.40	J/mol×K	680.01	Joback Method
cpg	269.17	J/mol×K	713.00	Joback Method

Sources

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=C14447155&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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