Cyanoacetic acid, hexyl ester

Inchi: InChI=1S/C9H15NO2/c1-2-3-4-5-8-12-9(11)6-7-10/h2-6,8H2,1H3
InchiKey: PWKKBTPSCGLYBR-UHFFFAOYSA-N
Formula: C9H15NO2
SMILES: CCCCCCOC(=O)CC#N
Mol. weight [g/mol]: 169.22

Physical Properties

Property code	Value	Unit	Source
gf	-75.84	kJ/mol	Joback Method
hf	-309.01	kJ/mol	Joback Method
hfus	23.36	kJ/mol	Joback Method
hvap	55.26	kJ/mol	Joback Method
log10ws	-2.32		Crippen Method
logp	2.024		Crippen Method
mcvol	146.490	ml/mol	McGowan Method
pc	2354.20	kPa	Joback Method
rinpol	1346.00		NIST Webbook
rinpol	1346.00		NIST Webbook
tb	583.69	K	Joback Method
tc	774.12	K	Joback Method
tf	328.34	K	Joback Method
vc	0.590	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	355.74	J/mol×K	583.69	Joback Method
cpg	367.30	J/mol×K	615.43	Joback Method
cpg	378.35	J/mol×K	647.17	Joback Method
cpg	388.88	J/mol×K	678.90	Joback Method
cpg	398.90	J/mol×K	710.64	Joback Method
cpg	408.42	J/mol×K	742.38	Joback Method
cpg	417.44	J/mol×K	774.12	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=U406223&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume