Cyanoacetic acid, nonyl ester

Inchi: InChI=1S/C12H21NO2/c1-2-3-4-5-6-7-8-11-15-12(14)9-10-13/h2-9,11H2,1H3
InchiKey: OTQOFAYPKSGELN-UHFFFAOYSA-N
Formula: C12H21NO2
SMILES: CCCCCCCCCOC(=O)CC#N
Mol. weight [g/mol]: 211.30

Physical Properties

Property code	Value	Unit	Source
gf	-50.58	kJ/mol	Joback Method
hf	-370.93	kJ/mol	Joback Method
hfus	31.13	kJ/mol	Joback Method
hvap	61.94	kJ/mol	Joback Method
log10ws	-3.57		Crippen Method
logp	3.194		Crippen Method
mcvol	188.760	ml/mol	McGowan Method
pc	1812.32	kPa	Joback Method
rinpol	1646.00		NIST Webbook
rinpol	1646.00		NIST Webbook
tb	652.33	K	Joback Method
tc	837.17	K	Joback Method
tf	362.15	K	Joback Method
vc	0.757	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	503.75	J/mol×K	652.33	Joback Method
cpg	517.43	J/mol×K	683.14	Joback Method
cpg	530.47	J/mol×K	713.94	Joback Method
cpg	542.86	J/mol×K	744.75	Joback Method
cpg	554.63	J/mol×K	775.56	Joback Method
cpg	565.78	J/mol×K	806.36	Joback Method
cpg	576.33	J/mol×K	837.17	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406226&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

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