Cyanoacetic acid, undecyl ester

Inchi: InChI=1S/C14H25NO2/c1-2-3-4-5-6-7-8-9-10-13-17-14(16)11-12-15/h2-11,13H2,1H3
InchiKey: MOHSIYYBSXQRJW-UHFFFAOYSA-N
Formula: C14H25NO2
SMILES: CCCCCCCCCCCOC(=O)CC#N
Mol. weight [g/mol]: 239.35

Physical Properties

Property code	Value	Unit	Source
gf	-33.74	kJ/mol	Joback Method
hf	-412.21	kJ/mol	Joback Method
hfus	36.31	kJ/mol	Joback Method
hvap	66.39	kJ/mol	Joback Method
log10ws	-4.41		Crippen Method
logp	3.974		Crippen Method
mcvol	216.940	ml/mol	McGowan Method
pc	1548.78	kPa	Joback Method
rinpol	1847.00		NIST Webbook
rinpol	1847.00		NIST Webbook
tb	698.09	K	Joback Method
tc	880.94	K	Joback Method
tf	384.69	K	Joback Method
vc	0.870	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	609.73	J/mol×K	698.09	Joback Method
cpg	624.49	J/mol×K	728.56	Joback Method
cpg	638.52	J/mol×K	759.04	Joback Method
cpg	651.84	J/mol×K	789.51	Joback Method
cpg	664.47	J/mol×K	819.99	Joback Method
cpg	676.41	J/mol×K	850.46	Joback Method
cpg	687.68	J/mol×K	880.94	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=U406228&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume