Cyanoacetic acid, tetradecyl ester

Inchi: InChI=1S/C17H31NO2/c1-2-3-4-5-6-7-8-9-10-11-12-13-16-20-17(19)14-15-18/h2-14,16H
InchiKey: KKUINEOCDWINEA-UHFFFAOYSA-N
Formula: C17H31NO2
SMILES: CCCCCCCCCCCCCCOC(=O)CC#N
Mol. weight [g/mol]: 281.43

Physical Properties

Property code	Value	Unit	Source
gf	-8.48	kJ/mol	Joback Method
hf	-474.13	kJ/mol	Joback Method
hfus	44.08	kJ/mol	Joback Method
hvap	73.07	kJ/mol	Joback Method
log10ws	-5.67		Crippen Method
logp	5.144		Crippen Method
mcvol	259.210	ml/mol	McGowan Method
pc	1249.49	kPa	Joback Method
rinpol	2152.00		NIST Webbook
rinpol	2152.00		NIST Webbook
tb	766.73	K	Joback Method
tc	950.19	K	Joback Method
tf	418.50	K	Joback Method
vc	1.038	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	777.89	J/mol×K	766.73	Joback Method
cpg	793.99	J/mol×K	797.31	Joback Method
cpg	809.25	J/mol×K	827.88	Joback Method
cpg	823.68	J/mol×K	858.46	Joback Method
cpg	837.31	J/mol×K	889.03	Joback Method
cpg	850.16	J/mol×K	919.61	Joback Method
cpg	862.25	J/mol×K	950.19	Joback Method

Sources

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=U406231&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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