Cyanoacetic acid, pentadecyl ester

Inchi: InChI=1S/C18H33NO2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-17-21-18(20)15-16-19/h2-15,1
InchiKey: VDBOSQXQWUTRGS-UHFFFAOYSA-N
Formula: C18H33NO2
SMILES: CCCCCCCCCCCCCCCOC(=O)CC#N
Mol. weight [g/mol]: 295.46

Physical Properties

Property code	Value	Unit	Source
gf	-0.06	kJ/mol	Joback Method
hf	-494.77	kJ/mol	Joback Method
hfus	46.67	kJ/mol	Joback Method
hvap	75.30	kJ/mol	Joback Method
log10ws	-6.09		Crippen Method
logp	5.534		Crippen Method
mcvol	273.300	ml/mol	McGowan Method
pc	1168.82	kPa	Joback Method
rinpol	2256.00		NIST Webbook
rinpol	2256.00		NIST Webbook
tb	789.61	K	Joback Method
tc	974.43	K	Joback Method
tf	429.77	K	Joback Method
vc	1.093	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	836.06	J/mol×K	789.61	Joback Method
cpg	852.58	J/mol×K	820.41	Joback Method
cpg	868.22	J/mol×K	851.22	Joback Method
cpg	882.98	J/mol×K	882.02	Joback Method
cpg	896.91	J/mol×K	912.83	Joback Method
cpg	910.02	J/mol×K	943.63	Joback Method
cpg	922.33	J/mol×K	974.43	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406232&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