Cyanoacetic acid, heptadecyl ester

Inchi: InChI=1S/C20H37NO2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-19-23-20(22)17-18-21/l
InchiKey: DEGKIJNOTWCZBX-UHFFFAOYSA-N
Formula: C20H37NO2
SMILES: CCCCCCCCCCCCCCCCCOC(=O)CC#N
Mol. weight [g/mol]: 323.51

Physical Properties

Property code	Value	Unit	Source
gf	16.78	kJ/mol	Joback Method
hf	-536.05	kJ/mol	Joback Method
hfus	51.85	kJ/mol	Joback Method
hvap	79.75	kJ/mol	Joback Method
log10ws	-6.92		Crippen Method
logp	6.315		Crippen Method
mcvol	301.480	ml/mol	McGowan Method
pc	1029.26	kPa	Joback Method
rinpol	2463.00		NIST Webbook
rinpol	2463.00		NIST Webbook
tb	835.37	K	Joback Method
tc	1025.02	K	Joback Method
tf	452.31	K	Joback Method
vc	1.206	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	955.13	J/mol×K	835.37	Joback Method
cpg	972.51	J/mol×K	866.98	Joback Method
cpg	988.90	J/mol×K	898.59	Joback Method
cpg	1004.33	J/mol×K	930.19	Joback Method
cpg	1018.83	J/mol×K	961.80	Joback Method
cpg	1032.42	J/mol×K	993.41	Joback Method
cpg	1045.14	J/mol×K	1025.02	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406234&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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