Cyanoacetic acid, dodecyl ester

Inchi: InChI=1S/C15H27NO2/c1-2-3-4-5-6-7-8-9-10-11-14-18-15(17)12-13-16/h2-12,14H2,1H3
InchiKey: RYFZYSKTNJAFQD-UHFFFAOYSA-N
Formula: C15H27NO2
SMILES: CCCCCCCCCCCCOC(=O)CC#N
Mol. weight [g/mol]: 253.38

Physical Properties

Property code	Value	Unit	Source
gf	-25.32	kJ/mol	Joback Method
hf	-432.85	kJ/mol	Joback Method
hfus	38.90	kJ/mol	Joback Method
hvap	68.62	kJ/mol	Joback Method
log10ws	-4.83		Crippen Method
logp	4.364		Crippen Method
mcvol	231.030	ml/mol	McGowan Method
pc	1438.07	kPa	Joback Method
rinpol	1948.00		NIST Webbook
rinpol	1948.00		NIST Webbook
tb	720.97	K	Joback Method
tc	903.49	K	Joback Method
tf	395.96	K	Joback Method
vc	0.925	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	664.65	J/mol×K	720.97	Joback Method
cpg	679.88	J/mol×K	751.39	Joback Method
cpg	694.34	J/mol×K	781.81	Joback Method
cpg	708.06	J/mol×K	812.23	Joback Method
cpg	721.05	J/mol×K	842.65	Joback Method
cpg	733.32	J/mol×K	873.07	Joback Method
cpg	744.90	J/mol×K	903.49	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406229&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