decyl 2-cyanoacrylate

Other names:	2-Propenoic acid, 2-cyano-, decyl ester
Inchi:	InChI=1S/C14H23NO2/c1-3-4-5-6-7-8-9-10-11-17-14(16)13(2)12-15/h2-11H2,1H3
InchiKey:	KWKVJEUILVQMRR-UHFFFAOYSA-N
Formula:	C14H23NO2
SMILES:	C=C(C#N)C(=O)OCCCCCCCCCC
Mol. weight [g/mol]:	237.34
CAS:	3578-07-2

Physical Properties

Property code	Value	Unit	Source
chl	-8380.60 ± 3.10	kJ/mol	NIST Webbook
gf	45.55	kJ/mol	Joback Method
hf	-296.57	kJ/mol	Joback Method
hfl	-415.60 ± 3.10	kJ/mol	NIST Webbook
hfus	33.72	kJ/mol	Joback Method
hvap	65.80	kJ/mol	Joback Method
log10ws	-4.27		Crippen Method
logp	3.750		Crippen Method
mcvol	212.640	ml/mol	McGowan Method
pc	1607.71	kPa	Joback Method
tb	694.65	K	Joback Method
tc	881.98	K	Joback Method
tf	368.97	K	Joback Method
vc	0.852	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	585.65	J/mol×K	694.65	Joback Method
cpg	600.01	J/mol×K	725.87	Joback Method
cpg	613.64	J/mol×K	757.09	Joback Method
cpg	626.55	J/mol×K	788.32	Joback Method
cpg	638.78	J/mol×K	819.54	Joback Method
cpg	650.32	J/mol×K	850.76	Joback Method

cpg	661.22	J/mol×K	881.98	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3578072&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

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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