Cyanoacetic acid, decyl ester

Inchi: InChI=1S/C13H23NO2/c1-2-3-4-5-6-7-8-9-12-16-13(15)10-11-14/h2-10,12H2,1H3
InchiKey: FEPOSCQQECTWHH-UHFFFAOYSA-N
Formula: C13H23NO2
SMILES: CCCCCCCCCCOC(=O)CC#N
Mol. weight [g/mol]: 225.33

Physical Properties

Property code	Value	Unit	Source
gf	-42.16	kJ/mol	Joback Method
hf	-391.57	kJ/mol	Joback Method
hfus	33.72	kJ/mol	Joback Method
hvap	64.17	kJ/mol	Joback Method
log10ws	-3.99		Crippen Method
logp	3.584		Crippen Method
mcvol	202.850	ml/mol	McGowan Method
pc	1672.79	kPa	Joback Method
rinpol	1748.00		NIST Webbook
rinpol	1748.00		NIST Webbook
tb	675.21	K	Joback Method
tc	858.85	K	Joback Method
tf	373.42	K	Joback Method
vc	0.814	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	556.07	J/mol×K	675.21	Joback Method
cpg	570.32	J/mol×K	705.82	Joback Method
cpg	583.88	J/mol×K	736.42	Joback Method
cpg	596.76	J/mol×K	767.03	Joback Method
cpg	608.98	J/mol×K	797.64	Joback Method
cpg	620.55	J/mol×K	828.24	Joback Method
cpg	631.48	J/mol×K	858.85	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406227&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