Cyanoacetic acid, octyl ester

Inchi: InChI=1S/C11H19NO2/c1-2-3-4-5-6-7-10-14-11(13)8-9-12/h2-8,10H2,1H3
InchiKey: MBCTWXWDQMXVDF-UHFFFAOYSA-N
Formula: C11H19NO2
SMILES: CCCCCCCCOC(=O)CC#N
Mol. weight [g/mol]: 197.27

Physical Properties

Property code	Value	Unit	Source
gf	-59.00	kJ/mol	Joback Method
hf	-350.29	kJ/mol	Joback Method
hfus	28.54	kJ/mol	Joback Method
hvap	59.71	kJ/mol	Joback Method
log10ws	-3.16		Crippen Method
logp	2.804		Crippen Method
mcvol	174.670	ml/mol	McGowan Method
pc	1970.05	kPa	Joback Method
rinpol	1547.00		NIST Webbook
tb	629.45	K	Joback Method
tc	815.85	K	Joback Method
tf	350.88	K	Joback Method
vc	0.702	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	452.85	J/mol×K	629.45	Joback Method
cpg	465.91	J/mol×K	660.52	Joback Method
cpg	478.36	J/mol×K	691.58	Joback Method
cpg	490.21	J/mol×K	722.65	Joback Method
cpg	501.47	J/mol×K	753.72	Joback Method
cpg	512.14	J/mol×K	784.79	Joback Method
cpg	522.25	J/mol×K	815.85	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406225&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