Acetic acid, cyano-, 2-ethylhexyl ester

Other names:	Cyanoacetic acid, 2-ethylhexyl ester
	2-Ethylhexyl cyanoacetate
	Ethylhexyl cyanoacetate
Inchi:	InChI=1S/C11H19NO2/c1-3-5-6-10(4-2)9-14-11(13)7-8-12/h10H,3-7,9H2,1-2H3
InchiKey:	ZNYBQVBNSXLZNI-UHFFFAOYSA-N
Formula:	C11H19NO2
SMILES:	CCCCC(CC)COC(=O)CC#N
Mol. weight [g/mol]:	197.27
CAS:	13361-34-7

Physical Properties

Property code	Value	Unit	Source
gf	-61.44	kJ/mol	Joback Method
hf	-355.57	kJ/mol	Joback Method
hfus	25.02	kJ/mol	Joback Method
hvap	59.33	kJ/mol	Joback Method
log10ws	-2.91		Crippen Method
logp	2.660		Crippen Method
mcvol	174.670	ml/mol	McGowan Method
pc	1984.12	kPa	Joback Method
tb	629.01	K	Joback Method
tc	818.64	K	Joback Method
tf	335.88	K	Joback Method
vc	0.696	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	453.31	J/mol×K	629.01	Joback Method
cpg	466.64	J/mol×K	660.61	Joback Method
cpg	479.33	J/mol×K	692.22	Joback Method
cpg	491.38	J/mol×K	723.82	Joback Method
cpg	502.82	J/mol×K	755.43	Joback Method
cpg	513.65	J/mol×K	787.03	Joback Method

cpg	523.87	J/mol×K	818.64	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13361347&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume