Cyanoacetic acid, 1-methylcyclohexyl, ethyl ester

Other names: Acetic acid, 2-cyano-2-(1-methylcyclohexyl), ethyl ester
Inchi: InChI=1S/C12H19NO2/c1-3-15-11(14)10(9-13)12(2)7-5-4-6-8-12/h10H,3-8H2,1-2H3
InchiKey: ROHCCJIABRKISQ-UHFFFAOYSA-N
Formula: C12H19NO2
SMILES: CCOC(=O)C(C#N)C1(C)CCCCC1
Mol. weight [g/mol]: 209.28

Physical Properties

Property code	Value	Unit	Source
gf	-34.06	kJ/mol	Joback Method
hf	-306.65	kJ/mol	Joback Method
hfus	13.14	kJ/mol	Joback Method
hvap	60.83	kJ/mol	Joback Method
log10ws	-2.99		Crippen Method
logp	2.660		Crippen Method
mcvol	177.900	ml/mol	McGowan Method
pc	2287.14	kPa	Joback Method
rinpol	1489.00		NIST Webbook
rinpol	1498.00		NIST Webbook
rinpol	1508.00		NIST Webbook
rinpol	1489.00		NIST Webbook
ripol	2005.00		NIST Webbook
ripol	2050.00		NIST Webbook
ripol	2005.00		NIST Webbook
ripol	2095.00		NIST Webbook
tb	671.68	K	Joback Method
tc	896.77	K	Joback Method
tf	378.43	K	Joback Method
vc	0.682	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	491.98	J/mol×K	671.68	Joback Method

cpg	508.34	J/mol×K	709.20	Joback Method
cpg	523.86	J/mol×K	746.71	Joback Method
cpg	538.64	J/mol×K	784.23	Joback Method
cpg	552.82	J/mol×K	821.74	Joback Method
cpg	566.49	J/mol×K	859.26	Joback Method
cpg	579.79	J/mol×K	896.77	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R97705&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume