

Cyclohexaneacetic acid, #-ethyl-, methyl ester

Other names:	M 3915
Inchi:	InChI=1S/C11H20O2/c1-3-10(11(12)13-2)9-7-5-4-6-8-9/h9-10H,3-8H2,1-2H3
InchiKey:	RCYYXYWVLKXHNT-UHFFFAOYSA-N
Formula:	C11H20O2
SMILES:	CCC(C(=O)OC)C1CCCCC1
Mol. weight [g/mol]:	184.28
CAS:	36613-93-1

Physical Properties

Property code	Value	Unit	Source
gf	-170.17	kJ/mol	Joback Method
hf	-466.13	kJ/mol	Joback Method
hfus	15.34	kJ/mol	Joback Method
hvap	49.28	kJ/mol	Joback Method
log10ws	-2.70		Crippen Method
logp	2.766		Crippen Method
mcvol	162.430	ml/mol	McGowan Method
pc	2462.92	kPa	Joback Method
tb	546.48	K	Joback Method
tc	753.14	K	Joback Method
tf	278.27	K	Joback Method
vc	0.603	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	404.33	J/molxK	546.48	Joback Method
cpg	423.31	J/molxK	580.92	Joback Method
cpg	441.31	J/molxK	615.37	Joback Method
cpg	458.33	J/molxK	649.81	Joback Method
cpg	474.40	J/molxK	684.25	Joback Method
cpg	489.53	J/molxK	718.70	Joback Method
cpg	503.73	J/molxK	753.14	Joback Method
dvisc	0.0057025	Paxs	278.27	Joback Method

dvisc	0.0022424	Paxs	322.97	Joback Method
dvisc	0.0011064	Paxs	367.67	Joback Method
dvisc	0.0006363	Paxs	412.38	Joback Method
dvisc	0.0004077	Paxs	457.08	Joback Method
dvisc	0.0002828	Paxs	501.78	Joback Method
dvisc	0.0002083	Paxs	546.48	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C36613931&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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

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