Cyclohexaneacetic acid, α-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	m3/kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0022424	Pa×s	322.97	Joback Method
dvisc	0.0011064	Pa×s	367.67	Joback Method
dvisc	0.0006363	Pa×s	412.38	Joback Method
dvisc	0.0004077	Pa×s	457.08	Joback Method
dvisc	0.0002828	Pa×s	501.78	Joback Method
dvisc	0.0002083	Pa×s	546.48	Joback Method

Sources

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
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
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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