

Cyclohexaneacetic acid, ethyl ester

Other names:	Ethyl cyclohexaneacetate Ethyl cyclohexylacetate Cyclohexylacetic acid ethyl ester
Inchi:	InChI=1S/C10H18O2/c1-2-12-10(11)8-9-6-4-3-5-7-9/h9H,2-8H2,1H3
InchiKey:	ZBDAMDWKXGTKBT-UHFFFAOYSA-N
Formula:	C10H18O2
SMILES:	CCOC(=O)CC1CCCCC1
Mol. weight [g/mol]:	170.25
CAS:	5452-75-5

Physical Properties

Property code	Value	Unit	Source
gf	-176.15	kJ/mol	Joback Method
hf	-440.21	kJ/mol	Joback Method
hfus	16.28	kJ/mol	Joback Method
hvap	47.44	kJ/mol	Joback Method
log10ws	-2.52		Crippen Method
logp	2.520		Crippen Method
mcvol	148.340	ml/mol	McGowan Method
pc	2693.00	kPa	Joback Method
tb	524.04	K	Joback Method
tc	729.39	K	Joback Method
tf	282.00	K	Joback Method
vc	0.552	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	355.31	J/molxK	524.04	Joback Method
cpg	373.16	J/molxK	558.27	Joback Method
cpg	390.11	J/molxK	592.49	Joback Method
cpg	406.18	J/molxK	626.72	Joback Method
cpg	421.39	J/molxK	660.94	Joback Method
cpg	435.73	J/molxK	695.17	Joback Method

cpg	449.24	J/mol×K	729.39	Joback Method
dvisc	0.0042103	Paxs	282.00	Joback Method
dvisc	0.0019412	Paxs	322.34	Joback Method
dvisc	0.0010632	Paxs	362.68	Joback Method
dvisc	0.0006569	Paxs	403.02	Joback Method
dvisc	0.0004431	Paxs	443.36	Joback Method
dvisc	0.0003191	Paxs	483.70	Joback Method
dvisc	0.0002418	Paxs	524.04	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5452755&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
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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