

Methylcyclohexylacetate

Other names:	Cyclohexaneacetic acid, methyl ester
Inchi:	InChI=1S/C9H16O2/c1-11-9(10)7-8-5-3-2-4-6-8/h8H,2-7H2,1H3
InchiKey:	IMXBRVLCKXGWSS-UHFFFAOYSA-N
Formula:	C9H16O2
SMILES:	COC(=O)CC1CCCCC1
Mol. weight [g/mol]:	156.22
CAS:	14352-61-5

Physical Properties

Property code	Value	Unit	Source
gf	-184.57	kJ/mol	Joback Method
hf	-419.57	kJ/mol	Joback Method
hfus	13.69	kJ/mol	Joback Method
hvap	45.21	kJ/mol	Joback Method
log10ws	-2.11		Crippen Method
logp	2.130		Crippen Method
mcvol	134.250	ml/mol	McGowan Method
pc	2982.79	kPa	Joback Method
tb	474.20	K	NIST Webbook
tc	709.61	K	Joback Method
tf	270.73	K	Joback Method
vc	0.496	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	308.34	J/molxK	501.16	Joback Method
cpg	325.39	J/molxK	535.90	Joback Method
cpg	341.59	J/molxK	570.64	Joback Method
cpg	356.96	J/molxK	605.38	Joback Method
cpg	371.51	J/molxK	640.12	Joback Method
cpg	385.24	J/molxK	674.87	Joback Method
cpg	398.17	J/molxK	709.61	Joback Method
dvisc	0.0043071	Paxs	270.73	Joback Method

dvisc	0.0020196	Paxs	309.13	Joback Method
dvisc	0.0011196	Paxs	347.54	Joback Method
dvisc	0.0006979	Paxs	385.94	Joback Method
dvisc	0.0004740	Paxs	424.35	Joback Method
dvisc	0.0003432	Paxs	462.75	Joback Method
dvisc	0.0002611	Paxs	501.16	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	365.70	K	2.00	NIST Webbook

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C14352615&Units=SI

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume

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