

Acetic acid, cis-4-methylcyclohexyl ester

Inchi:	InChI=1S/C9H16O2/c1-7-3-5-9(6-4-7)11-8(2)10/h7,9H,3-6H2,1-2H3
InchiKey:	VJBFCCCTSQEGMH-UHFFFAOYSA-N
Formula:	C9H16O2
SMILES:	CC(=O)OC1CCC(C)CC1
Mol. weight [g/mol]:	156.22

Physical Properties

Property code	Value	Unit	Source
gf	-192.28	kJ/mol	Joback Method
hf	-439.91	kJ/mol	Joback Method
hfus	14.76	kJ/mol	Joback Method
hvap	44.90	kJ/mol	Joback Method
log10ws	-2.22		Crippen Method
logp	2.128		Crippen Method
mcvol	134.250	ml/mol	McGowan Method
pc	2878.12	kPa	Joback Method
rinpol	1111.00		NIST Webbook
tb	496.49	K	Joback Method
tc	704.73	K	Joback Method
tf	266.49	K	Joback Method
vc	0.495	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	308.98	J/molxK	496.49	Joback Method
cpg	387.96	J/molxK	670.02	Joback Method
cpg	373.79	J/molxK	635.31	Joback Method
cpg	358.81	J/molxK	600.61	Joback Method
cpg	343.02	J/molxK	565.90	Joback Method
cpg	326.41	J/molxK	531.20	Joback Method
cpg	401.32	J/molxK	704.73	Joback Method
dvisc	0.0002776	Paxs	496.49	Joback Method
dvisc	0.0003516	Paxs	458.16	Joback Method

dvisc	0.0004650	Paxs	419.82	Joback Method
dvisc	0.0006505	Paxs	381.49	Joback Method
dvisc	0.0009810	Paxs	343.16	Joback Method
dvisc	0.0016403	Paxs	304.82	Joback Method
dvisc	0.0031798	Paxs	266.49	Joback Method

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=U368248&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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