

Acetic acid

4,5-dimethoxy-tetrahydro-pyran-3-yl ester

Inchi:	InChI=1S/C9H16O5/c1-6(10)14-8-5-13-4-7(11-2)9(8)12-3/h7-9H,4-5H2,1-3H3
InchiKey:	NFTACBULRBCFQP-UHFFFAOYSA-N
Formula:	C9H16O5
SMILES:	COC1COCC(OC(C)=O)C1OC
Mol. weight [g/mol]:	204.22

Physical Properties

Property code	Value	Unit	Source
gf	-496.11	kJ/mol	Joback Method
hf	-856.69	kJ/mol	Joback Method
hfus	26.19	kJ/mol	Joback Method
hvap	53.92	kJ/mol	Joback Method
log10ws	0.06		Crippen Method
logp	-0.022		Crippen Method
mcvol	151.860	ml/mol	McGowan Method
pc	2657.03	kPa	Joback Method
rinpol	1318.76		NIST Webbook
tb	563.61	K	Joback Method
tc	766.45	K	Joback Method
tf	333.28	K	Joback Method
vc	0.551	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	394.65	J/molxK	563.61	Joback Method
cpg	411.26	J/molxK	597.42	Joback Method
cpg	427.15	J/molxK	631.22	Joback Method
cpg	442.31	J/molxK	665.03	Joback Method
cpg	456.70	J/molxK	698.84	Joback Method
cpg	470.29	J/molxK	732.64	Joback Method
cpg	483.06	J/molxK	766.45	Joback Method
dvisc	0.0015574	Paxs	333.28	Joback Method
dvisc	0.0009409	Paxs	371.67	Joback Method

dvisc	0.0006247	Paxs	410.06	Joback Method
dvisc	0.0004449	Paxs	448.44	Joback Method
dvisc	0.0003342	Paxs	486.83	Joback Method
dvisc	0.0002618	Paxs	525.22	Joback Method
dvisc	0.0002121	Paxs	563.61	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R268138&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
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
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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