

Methyldicyclopropylglycolate

Inchi:	InChI=1S/C9H14O3/c1-12-8(10)9(11,6-2-3-6)7-4-5-7/h6-7,11H,2-5H2,1H3
InchiKey:	OGSXJBVCOSDQU-UHFFFAOYSA-N
Formula:	C9H14O3
SMILES:	COC(=O)C(O)(C1CC1)C1CC1
Mol. weight [g/mol]:	170.21
CAS:	100144-93-2

Physical Properties

Property code	Value	Unit	Source
gf	-221.50	kJ/mol	Joback Method
hf	-489.27	kJ/mol	Joback Method
hfus	14.80	kJ/mol	Joback Method
hvap	59.99	kJ/mol	Joback Method
log10ws	-1.13		Crippen Method
logp	0.710		Crippen Method
mcvol	129.260	ml/mol	McGowan Method
pc	3607.21	kPa	Joback Method
tb	584.04	K	Joback Method
tc	784.19	K	Joback Method
tf	362.47	K	Joback Method
vc	0.485	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	354.20	J/mol×K	584.04	Joback Method
cpg	367.27	J/mol×K	617.40	Joback Method
cpg	379.44	J/mol×K	650.76	Joback Method
cpg	390.79	J/mol×K	684.12	Joback Method
cpg	401.39	J/mol×K	717.47	Joback Method
cpg	411.31	J/mol×K	750.83	Joback Method
cpg	420.62	J/mol×K	784.19	Joback Method
dvisc	0.0055827	Pa×s	362.47	Joback Method
dvisc	0.0029848	Pa×s	399.40	Joback Method

dvisc	0.0017743	Pa×s	436.33	Joback Method
dvisc	0.0011439	Pa×s	473.25	Joback Method
dvisc	0.0007858	Pa×s	510.18	Joback Method
dvisc	0.0005679	Pa×s	547.11	Joback Method
dvisc	0.0004277	Pa×s	584.04	Joback Method

Sources

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=C100144932&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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