1,3-Propanediol, 2-methyl-, diacetate

Inchi: InChI=1S/C8H14O4/c1-6(4-11-7(2)9)5-12-8(3)10/h6H,4-5H2,1-3H3
InchiKey: ODKLKBUOGOLEJW-UHFFFAOYSA-N
Formula: C8H14O4
SMILES: CC(=O)OCC(C)COC(C)=O
Mol. weight [g/mol]: 174.19
CAS: 55289-53-7

Physical Properties

Property code	Value	Unit	Source
gf	-453.80	kJ/mol	Joback Method
hf	-703.33	kJ/mol	Joback Method
hfus	18.53	kJ/mol	Joback Method
hvap	51.33	kJ/mol	Joback Method
log10ws	-0.65		Crippen Method
logp	0.749		Crippen Method
mcvol	138.460	ml/mol	McGowan Method
pc	2811.36	kPa	Joback Method
tb	534.58	K	Joback Method
tc	722.01	K	Joback Method
tf	309.24	K	Joback Method
vc	0.525	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	322.54	J/mol×K	534.58	Joback Method
cpg	376.76	J/mol×K	690.77	Joback Method
cpg	366.85	J/mol×K	659.53	Joback Method
cpg	356.46	J/mol×K	628.29	Joback Method
cpg	345.61	J/mol×K	597.06	Joback Method
cpg	334.30	J/mol×K	565.82	Joback Method
cpg	386.20	J/mol×K	722.01	Joback Method
dvisc	0.0002153	Pa×s	534.58	Joback Method
dvisc	0.0002792	Pa×s	497.02	Joback Method

dvisc	0.0003777	Pa×s	459.47	Joback Method
dvisc	0.0005393	Pa×s	421.91	Joback Method
dvisc	0.0008255	Pa×s	384.35	Joback Method
dvisc	0.0013856	Pa×s	346.80	Joback Method
dvisc	0.0026376	Pa×s	309.24	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=C55289537&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