1,3-Propanediol diisobutyrate, 2,2-dimethyl

Other names: 2,2-dimethylpropane-1,3-diyl bisisobutyrate
Inchi: InChI=1S/C13H24O4/c1-9(2)11(14)16-7-13(5,6)8-17-12(15)10(3)4/h9-10H,7-8H2,1-6H3
InchiKey: HACYJIJMLQDPDS-UHFFFAOYSA-N
Formula: C13H24O4
SMILES: CC(C)C(=O)OCC(C)(C)COC(=O)C(C)C
Mol. weight [g/mol]: 244.33
CAS: 63512-34-5

Physical Properties

Property code	Value	Unit	Source
gf	-411.30	kJ/mol	Joback Method
hf	-820.56	kJ/mol	Joback Method
hfus	20.54	kJ/mol	Joback Method
hvap	60.77	kJ/mol	Joback Method
log10ws	-2.26		Crippen Method
logp	2.411		Crippen Method
mcvol	208.910	ml/mol	McGowan Method
pc	1827.85	kPa	Joback Method
tb	645.31	K	Joback Method
tc	835.59	K	Joback Method
tf	353.01	K	Joback Method
vc	0.788	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	572.06	J/mol×K	645.31	Joback Method
cpg	588.28	J/mol×K	677.02	Joback Method
cpg	603.65	J/mol×K	708.74	Joback Method
cpg	618.18	J/mol×K	740.45	Joback Method
cpg	631.88	J/mol×K	772.16	Joback Method
cpg	644.77	J/mol×K	803.87	Joback Method
cpg	656.88	J/mol×K	835.59	Joback Method
dvisc	0.0028022	Pa×s	353.01	Joback Method

dvisc	0.0011521	Pa×s	401.73	Joback Method
dvisc	0.0005741	Pa×s	450.44	Joback Method
dvisc	0.0003278	Pa×s	499.16	Joback Method
dvisc	0.0002067	Pa×s	547.88	Joback Method
dvisc	0.0001406	Pa×s	596.59	Joback Method
dvisc	0.0001013	Pa×s	645.31	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C63512345&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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume