threo-butane-2,3-diol diacetate

Other names: 2,3-Butanediol, diacetate, rac
Inchi: InChI=1S/C8H14O4/c1-5(11-7(3)9)6(2)12-8(4)10/h5-6H,1-4H3/t5-,6-/m1/s1
InchiKey: VVSAAKSQXNXBML-PHDIDXHHSA-N
Formula: C8H14O4
SMILES: CC(=O)OC(C)C(C)OC(C)=O
Mol. weight [g/mol]: 174.19

Physical Properties

Property code	Value	Unit	Source
gf	-456.24	kJ/mol	Joback Method
hf	-708.61	kJ/mol	Joback Method
hfus	15.00	kJ/mol	Joback Method
hvap	50.94	kJ/mol	Joback Method
log10ws	-1.12		Crippen Method
logp	0.890		Crippen Method
mcvol	138.460	ml/mol	McGowan Method
pc	2835.36	kPa	Joback Method
rinpol	1054.00		NIST Webbook
rinpol	1054.00		NIST Webbook
ripol	1521.00		NIST Webbook
ripol	1521.00		NIST Webbook
tb	534.14	K	Joback Method
tc	725.42	K	Joback Method
tf	294.24	K	Joback Method
vc	0.519	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	322.86	J/mol×K	534.14	Joback Method
cpg	378.34	J/mol×K	693.54	Joback Method
cpg	368.23	J/mol×K	661.66	Joback Method
cpg	357.62	J/mol×K	629.78	Joback Method
cpg	346.52	J/mol×K	597.90	Joback Method

cpg	334.93	J/mol×K	566.02	Joback Method
cpg	387.93	J/mol×K	725.42	Joback Method
dvisc	0.0002027	Pa×s	534.14	Joback Method
dvisc	0.0002693	Pa×s	494.16	Joback Method
dvisc	0.0003762	Pa×s	454.17	Joback Method
dvisc	0.0005605	Pa×s	414.19	Joback Method
dvisc	0.0009094	Pa×s	374.21	Joback Method
dvisc	0.0016565	Pa×s	334.22	Joback Method
dvisc	0.0035516	Pa×s	294.24	Joback Method

Sources

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=R319652&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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