1,2,4-Butanetriol, triacetate

Other names: butane-1,2,4-triol, acetylated
Inchi: InChI=1S/C10H16O6/c1-7(11)14-5-4-10(16-9(3)13)6-15-8(2)12/h10H,4-6H2,1-3H3
InchiKey: RPOOYSKKKVGNAP-UHFFFAOYSA-N
Formula: C10H16O6
SMILES: CC(=O)OCCC(COC(C)=O)OC(C)=O
Mol. weight [g/mol]: 232.23
CAS: 14835-47-3

Physical Properties

Property code	Value	Unit	Source
gf	-670.88	kJ/mol	Joback Method
hf	-989.41	kJ/mol	Joback Method
hfus	26.49	kJ/mol	Joback Method
hvap	64.93	kJ/mol	Joback Method
log10ws	-0.71		Crippen Method
logp	0.434		Crippen Method
mcvol	174.080	ml/mol	McGowan Method
pc	2421.88	kPa	Joback Method
rinpol	1399.20		NIST Webbook
rinpol	1399.20		NIST Webbook
tb	656.63	K	Joback Method
tc	846.48	K	Joback Method
tf	403.94	K	Joback Method
vc	0.661	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	459.50	J/mol×K	656.63	Joback Method
cpg	471.88	J/mol×K	688.27	Joback Method
cpg	483.64	J/mol×K	719.91	Joback Method
cpg	494.77	J/mol×K	751.55	Joback Method
cpg	505.25	J/mol×K	783.20	Joback Method
cpg	515.07	J/mol×K	814.84	Joback Method

cpg	524.20	J/mol×K	846.48	Joback Method
dvisc	0.0013591	Pa×s	403.94	Joback Method
dvisc	0.0007766	Pa×s	446.06	Joback Method
dvisc	0.0004887	Pa×s	488.17	Joback Method
dvisc	0.0003310	Pa×s	530.28	Joback Method
dvisc	0.0002374	Pa×s	572.40	Joback Method
dvisc	0.0001782	Pa×s	614.51	Joback Method
dvisc	0.0001388	Pa×s	656.63	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C14835473&Units=SI
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

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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