

(S)-(-)-1,2,4-Butanetriol, 2,4-di(acetate)

Inchi:	InChI=1S/C8H14O5/c1-6(10)12-4-3-8(5-9)13-7(2)11/h8-9H,3-5H2,1-2H3
InchiKey:	WJPFWMOVDNJVNE-UHFFFAOYSA-N
Formula:	C8H14O5
SMILES:	CC(=O)OCCC(CO)OC(C)=O
Mol. weight [g/mol]:	190.19

Physical Properties

Property code	Value	Unit	Source
gf	-590.62	kJ/mol	Joback Method
hf	-855.56	kJ/mol	Joback Method
hfus	22.62	kJ/mol	Joback Method
hvap	68.00	kJ/mol	Joback Method
log10ws	-0.27		Crippen Method
logp	-0.136		Crippen Method
mcvol	144.330	ml/mol	McGowan Method
pc	3107.10	kPa	Joback Method
rinpol	1445.00		NIST Webbook
tb	626.76	K	Joback Method
tc	805.81	K	Joback Method
tf	370.06	K	Joback Method
vc	0.544	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	373.00	J/molxK	626.76	Joback Method
cpg	383.17	J/molxK	656.60	Joback Method
cpg	392.88	J/molxK	686.44	Joback Method
cpg	402.14	J/molxK	716.29	Joback Method
cpg	410.94	J/molxK	746.13	Joback Method
cpg	419.27	J/molxK	775.97	Joback Method
cpg	427.12	J/molxK	805.81	Joback Method
dvisc	0.0032891	Paxs	370.06	Joback Method
dvisc	0.0012145	Paxs	412.84	Joback Method

dvisc	0.0005407	Paxs	455.63	Joback Method
dvisc	0.0002766	Paxs	498.41	Joback Method
dvisc	0.0001573	Paxs	541.19	Joback Method
dvisc	0.0000972	Paxs	583.98	Joback Method
dvisc	0.0000641	Paxs	626.76	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=U374867&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
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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