

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

Inchi:	InChI=1S/C6H12O4/c1-5(9)10-6(4-8)2-3-7/h6-8H,2-4H2,1H3
InchiKey:	SDDGXTZPTOYNOA-UHFFFAOYSA-N
Formula:	C6H12O4
SMILES:	CC(=O)OC(CO)CCO
Mol. weight [g/mol]:	148.16

Physical Properties

Property code	Value	Unit	Source
gf	-510.36	kJ/mol	Joback Method
hf	-721.71	kJ/mol	Joback Method
hfus	18.74	kJ/mol	Joback Method
hvap	71.08	kJ/mol	Joback Method
log10ws	0.16		Crippen Method
logp	-0.707		Crippen Method
mcvol	114.580	ml/mol	McGowan Method
pc	4130.29	kPa	Joback Method
rinpol	1247.00		NIST Webbook
tb	596.89	K	Joback Method
tc	765.41	K	Joback Method
tf	336.18	K	Joback Method
vc	0.427	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	290.26	J/molxK	596.89	Joback Method
cpg	298.25	J/molxK	624.98	Joback Method
cpg	305.91	J/molxK	653.06	Joback Method
cpg	313.24	J/molxK	681.15	Joback Method
cpg	320.25	J/molxK	709.24	Joback Method
cpg	326.94	J/molxK	737.33	Joback Method
cpg	333.30	J/molxK	765.41	Joback Method
dvisc	0.0159133	Paxs	336.18	Joback Method
dvisc	0.0031897	Paxs	379.63	Joback Method

dvisc	0.0008894	Paxs	423.08	Joback Method
dvisc	0.0003146	Paxs	466.53	Joback Method
dvisc	0.0001329	Paxs	509.99	Joback Method
dvisc	0.0000642	Paxs	553.44	Joback Method
dvisc	0.0000345	Paxs	596.89	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U374866&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
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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