

2,3-Butanediol, monoacetate, threo

Inchi:	InChI=1S/C6H12O3/c1-4(7)5(2)9-6(3)8/h4-5,7H,1-3H3/t4-,5-/m1/s1
InchiKey:	BCWWODMTUXMSAB-RFZPGFLSSA-N
Formula:	C6H12O3
SMILES:	CC(=O)OC(C)C(C)O
Mol. weight [g/mol]:	132.16

Physical Properties

Property code	Value	Unit	Source
gf	-375.98	kJ/mol	Joback Method
hf	-574.76	kJ/mol	Joback Method
hfus	11.12	kJ/mol	Joback Method
hvap	54.01	kJ/mol	Joback Method
log10ws	-0.68		Crippen Method
logp	0.319		Crippen Method
mcvol	108.710	ml/mol	McGowan Method
pc	3718.02	kPa	Joback Method
ripol	1594.00		NIST Webbook
ripol	1594.00		NIST Webbook
tb	504.27	K	Joback Method
tc	682.14	K	Joback Method
tf	260.36	K	Joback Method
vc	0.403	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	246.04	J/molxK	504.27	Joback Method
cpg	289.19	J/molxK	652.50	Joback Method
cpg	281.27	J/molxK	622.85	Joback Method
cpg	272.99	J/molxK	593.21	Joback Method
cpg	264.36	J/molxK	563.56	Joback Method
cpg	255.38	J/molxK	533.92	Joback Method
cpg	296.77	J/molxK	682.14	Joback Method
dvisc	0.0001409	Paxs	504.27	Joback Method

dvisc	0.0002390	Paxs	463.62	Joback Method
dvisc	0.0004487	Paxs	422.97	Joback Method
dvisc	0.0009632	Paxs	382.31	Joback Method
dvisc	0.0024799	Paxs	341.66	Joback Method
dvisc	0.0082434	Paxs	301.01	Joback Method
dvisc	0.0398736	Paxs	260.36	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R616394&Units=SI
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

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

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