3-acetoxy-2-butanol (2)

Other names: threo-3-acetoxy-2-butanol
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
rinpol	932.00		NIST Webbook
rinpol	932.00		NIST Webbook
ripol	1576.00		NIST Webbook
ripol	1597.00		NIST Webbook
ripol	1597.00		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/mol×K	504.27	Joback Method
cpg	255.38	J/mol×K	533.92	Joback Method
cpg	264.36	J/mol×K	563.56	Joback Method

cpg	272.99	J/mol×K	593.21	Joback Method
cpg	281.27	J/mol×K	622.85	Joback Method
cpg	289.19	J/mol×K	652.50	Joback Method
cpg	296.77	J/mol×K	682.14	Joback Method
dvisc	0.0398736	Pa×s	260.36	Joback Method
dvisc	0.0082434	Pa×s	301.01	Joback Method
dvisc	0.0024799	Pa×s	341.66	Joback Method
dvisc	0.0009632	Pa×s	382.31	Joback Method
dvisc	0.0004487	Pa×s	422.97	Joback Method
dvisc	0.0002390	Pa×s	463.62	Joback Method
dvisc	0.0001409	Pa×s	504.27	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R319647&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

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