3-acetoxy-2-butanol (1)

Other names: erythro-3-acetoxy-2-butanol
Inchi: InChI=1S/C6H12O3/c1-4(7)5(2)9-6(3)8/h4-5,7H,1-3H3/t4-,5+/m1/s1
InchiKey: BCWWODMTUXMSAB-UHNVWZDZSA-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	1581.00		NIST Webbook
ripol	1563.00		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

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R319523&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume