2-Butene-1,4-diol, diacetate

Other names: 2-Buten-1,4-diol, diacetate
4-(Acetyloxy)-2-butenyl acetate
2-Butene-1,4-diol, 1,4-diacetate
Inchi: InChI=1S/C8H12O4/c1-7(9)11-5-3-4-6-12-8(2)10/h3-4H,5-6H2,1-2H3/b4-3+
InchiKey: VZUAUHWZIKOMFC-ONEGZZNKSA-N
Formula: C8H12O4
SMILES: CC(=O)OCC=CCOC(C)=O
Mol. weight [g/mol]: 172.18
CAS: 18621-75-5

Physical Properties

Property code	Value	Unit	Source
gf	-371.14	kJ/mol	Joback Method
hf	-580.83	kJ/mol	Joback Method
hfus	22.25	kJ/mol	Joback Method
hvap	51.67	kJ/mol	Joback Method
log10ws	-0.75		Crippen Method
logp	0.669		Crippen Method
mcvol	134.160	ml/mol	McGowan Method
pc	2947.28	kPa	Joback Method
rinpol	1253.00		NIST Webbook
tb	539.18	K	Joback Method
tc	730.81	K	Joback Method
tf	319.16	K	Joback Method
vc	0.511	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	303.47	J/mol×K	539.18	Joback Method
cpg	314.43	J/mol×K	571.12	Joback Method
cpg	324.91	J/mol×K	603.06	Joback Method
cpg	334.94	J/mol×K	634.99	Joback Method
cpg	344.49	J/mol×K	666.93	Joback Method

cpg	353.58	J/mol×K	698.87	Joback Method
cpg	362.20	J/mol×K	730.81	Joback Method
dvisc	0.0018749	Pa×s	319.16	Joback Method
dvisc	0.0010564	Pa×s	355.83	Joback Method
dvisc	0.0006626	Pa×s	392.50	Joback Method
dvisc	0.0004501	Pa×s	429.17	Joback Method
dvisc	0.0003249	Pa×s	465.84	Joback Method
dvisc	0.0002460	Pa×s	502.51	Joback Method
dvisc	0.0001934	Pa×s	539.18	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=C18621755&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