1,3-Butanediol, diacetate

Other names:	1,3-Butylene diacetate
	1,3-Butylene glycol diacetate
	1,3-Diacetoxybutane
	1,3-Butandiol diacetate
Inchi:	InChI=1S/C8H14O4/c1-6(12-8(3)10)4-5-11-7(2)9/h6H,4-5H2,1-3H3
InchiKey:	MPAGVACEWQNVQO-UHFFFAOYSA-N
Formula:	C8H14O4
SMILES:	CC(=O)OCCC(C)OC(C)=O
Mol. weight [g/mol]:	174.19
CAS:	1117-31-3

Physical Properties

Property code	Value	Unit	Source
gf	-453.80	kJ/mol	Joback Method
hf	-703.33	kJ/mol	Joback Method
hfus	18.53	kJ/mol	Joback Method
hvap	51.33	kJ/mol	Joback Method
log10ws	-1.01		Crippen Method
logp	0.891		Crippen Method
mcvol	138.460	ml/mol	McGowan Method
pc	2811.36	kPa	Joback Method
rinpol	1123.70		NIST Webbook
rinpol	1123.70		NIST Webbook
tb	534.58	K	Joback Method
tc	722.01	K	Joback Method
tf	309.24	K	Joback Method
vc	0.525	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	322.54	J/mol×K	534.58	Joback Method
cpg	334.30	J/mol×K	565.82	Joback Method
cpg	345.61	J/mol×K	597.06	Joback Method

cpg	356.46	J/mol×K	628.29	Joback Method
cpg	366.85	J/mol×K	659.53	Joback Method
cpg	376.76	J/mol×K	690.77	Joback Method
cpg	386.20	J/mol×K	722.01	Joback Method
dvisc	0.0026376	Pa×s	309.24	Joback Method
dvisc	0.0013856	Pa×s	346.80	Joback Method
dvisc	0.0008255	Pa×s	384.35	Joback Method
dvisc	0.0005393	Pa×s	421.91	Joback Method
dvisc	0.0003777	Pa×s	459.47	Joback Method
dvisc	0.0002792	Pa×s	497.02	Joback Method
dvisc	0.0002153	Pa×s	534.58	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	371.20	K	1.00	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1117313&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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume