

2,3-Butanediol, diacetate

Other names:	2,3-Butanediyl diacetate Butane-2,3-diol, diacetate 2,3-Diacetoxybutane butane-2,3-diyl diacetate
Inchi:	InChI=1S/C8H14O4/c1-5(11-7(3)9)6(2)12-8(4)10/h5-6H,1-4H3
InchiKey:	VVSAAKSQXNXBML-UHFFFAOYSA-N
Formula:	C8H14O4
SMILES:	CC(=O)OC(C)C(C)OC(C)=O
Mol. weight [g/mol]:	174.19
CAS:	1114-92-7

Physical Properties

Property code	Value	Unit	Source
gf	-456.24	kJ/mol	Joback Method
hf	-708.61	kJ/mol	Joback Method
hfl	-916.30 ± 3.30	kJ/mol	NIST Webbook
hfus	15.00	kJ/mol	Joback Method
hvap	50.94	kJ/mol	Joback Method
log10ws	-1.12		Crippen Method
logp	0.890		Crippen Method
mcvol	138.460	ml/mol	McGowan Method
pc	2835.36	kPa	Joback Method
rinpol	1064.00		NIST Webbook
rinpol	1065.40		NIST Webbook
rinpol	1080.00		NIST Webbook
rinpol	1065.40		NIST Webbook
rinpol	1080.00		NIST Webbook
ripol	1487.00		NIST Webbook
ripol	1521.00		NIST Webbook
ripol	1484.00		NIST Webbook
ripol	1501.00		NIST Webbook
ripol	1484.00		NIST Webbook
ripol	1483.00		NIST Webbook
ripol	1532.00		NIST Webbook
ripol	1495.00		NIST Webbook
ripol	1525.00		NIST Webbook
tb	534.14	K	Joback Method

tc	725.42	K	Joback Method
tf	294.24	K	Joback Method
vc	0.519	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	322.86	J/mol×K	534.14	Joback Method
cpg	334.93	J/mol×K	566.02	Joback Method
cpg	346.52	J/mol×K	597.90	Joback Method
cpg	357.62	J/mol×K	629.78	Joback Method
cpg	368.23	J/mol×K	661.66	Joback Method
cpg	378.34	J/mol×K	693.54	Joback Method
cpg	387.93	J/mol×K	725.42	Joback Method
dvisc	0.0035516	Pa×s	294.24	Joback Method
dvisc	0.0016565	Pa×s	334.22	Joback Method
dvisc	0.0009094	Pa×s	374.21	Joback Method
dvisc	0.0005605	Pa×s	414.19	Joback Method
dvisc	0.0003762	Pa×s	454.17	Joback Method
dvisc	0.0002693	Pa×s	494.16	Joback Method
dvisc	0.0002027	Pa×s	534.14	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1114927&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

hfl:	Liquid phase 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

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