

cis-1,4-Diacetoxy-2-butene

Other names:	2-Butene-1,4-diol, 1,4-diacetate, (2Z)- cis-1,4-Diacetoxy-2-buten
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-ARJAWSKDSA-N
Formula:	C8H12O4
SMILES:	CC(=O)OCC=CCOC(C)=O
Mol. weight [g/mol]:	172.18
CAS:	25260-60-0

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
mvol	134.160	ml/mol	McGowan Method
pc	2947.28	kPa	Joback Method
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/molxK	539.18	Joback Method
cpg	314.43	J/molxK	571.12	Joback Method
cpg	324.91	J/molxK	603.06	Joback Method
cpg	334.94	J/molxK	634.99	Joback Method
cpg	344.49	J/molxK	666.93	Joback Method
cpg	353.58	J/molxK	698.87	Joback Method
cpg	362.20	J/molxK	730.81	Joback Method

dvisc	0.0018749	Paxs	319.16	Joback Method
dvisc	0.0010564	Paxs	355.83	Joback Method
dvisc	0.0006626	Paxs	392.50	Joback Method
dvisc	0.0004501	Paxs	429.17	Joback Method
dvisc	0.0003249	Paxs	465.84	Joback Method
dvisc	0.0002460	Paxs	502.51	Joback Method
dvisc	0.0001934	Paxs	539.18	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C25260600&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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