1,2-Diacetoxy-3-(2-methoxyphenoxy)propane

Other names: Guaifenesin, acetylated
Inchi: InChI=1S/C14H18O6/c1-10(15)18-8-12(20-11(2)16)9-19-14-7-5-4-6-13(14)17-3/h4-7,12H
InchiKey: HPQAMKIXSOVULB-UHFFFAOYSA-N
Formula: C14H18O6
SMILES: COc1ccccc1OCC(COC(C)=O)OC(C)=O
Mol. weight [g/mol]: 282.29
CAS: 92865-65-1

Physical Properties

Property code	Value	Unit	Source
gf	-510.50	kJ/mol	Joback Method
hf	-866.55	kJ/mol	Joback Method
hfus	30.09	kJ/mol	Joback Method
hvap	72.44	kJ/mol	Joback Method
log10ws	-2.06		Crippen Method
logp	1.569		Crippen Method
mcvol	210.980	ml/mol	McGowan Method
pc	2104.20	kPa	Joback Method
rinpol	1865.00		NIST Webbook
rinpol	1865.00		NIST Webbook
tb	748.36	K	Joback Method
tc	954.66	K	Joback Method
tf	460.26	K	Joback Method
vc	0.789	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	593.96	J/mol×K	748.36	Joback Method
cpg	607.92	J/mol×K	782.74	Joback Method
cpg	620.90	J/mol×K	817.13	Joback Method
cpg	632.88	J/mol×K	851.51	Joback Method
cpg	643.84	J/mol×K	885.89	Joback Method
cpg	653.75	J/mol×K	920.28	Joback Method

cpg	662.60	J/mol×K	954.66	Joback Method
dvisc	0.0005860	Pa×s	460.26	Joback Method
dvisc	0.0003416	Pa×s	508.28	Joback Method
dvisc	0.0002186	Pa×s	556.29	Joback Method
dvisc	0.0001501	Pa×s	604.31	Joback Method
dvisc	0.0001090	Pa×s	652.33	Joback Method
dvisc	0.0000827	Pa×s	700.34	Joback Method
dvisc	0.0000650	Pa×s	748.36	Joback Method

Sources

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=C92865651&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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