Benzal diacetate

Other names:	Methanediol, phenyl-, diacetate
	Phenylmethanediol diacetate
	Benzylidene diacetate
Inchi:	InChI=1S/C11H12O4/c1-8(12)14-11(15-9(2)13)10-6-4-3-5-7-10/h3-7,11H,1-2H3
InchiKey:	XRYSDRCNTMEYFH-UHFFFAOYSA-N
Formula:	C11H12O4
SMILES:	CC(=O)OC(OC(C)=O)c1ccccc1
Mol. weight [g/mol]:	208.21
CAS:	581-55-5

Physical Properties

Property code	Value	Unit	Source
chs	-5270.56 ± 0.57	kJ/mol	NIST Webbook
gf	-316.13	kJ/mol	Joback Method
hf	-676.85 ± 0.99	kJ/mol	NIST Webbook
hfs	-773.02 ± 0.57	kJ/mol	NIST Webbook
hfus	20.34	kJ/mol	Joback Method
hsub	96.20	kJ/mol	NIST Webbook
hsub	96.17 ± 0.84	kJ/mol	NIST Webbook
hvap	60.28	kJ/mol	Joback Method
log10ws	-2.21		Crippen Method
logp	1.811		Crippen Method
mcvol	156.970	ml/mol	McGowan Method
pc	2944.08	kPa	Joback Method
rinpol	1322.30		NIST Webbook
rinpol	1321.00		NIST Webbook
rinpol	1321.00		NIST Webbook
tb	629.90	K	Joback Method
tc	848.60	K	Joback Method
tf	369.47	K	Joback Method
vc	0.586	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	388.35	J/mol×K	629.90	Joback Method
cpg	401.53	J/mol×K	666.35	Joback Method
cpg	413.88	J/mol×K	702.80	Joback Method
cpg	425.39	J/mol×K	739.25	Joback Method
cpg	436.08	J/mol×K	775.70	Joback Method
cpg	445.94	J/mol×K	812.15	Joback Method
cpg	454.98	J/mol×K	848.60	Joback Method
dvisc	0.0017390	Pa×s	369.47	Joback Method
dvisc	0.0009421	Pa×s	412.88	Joback Method
dvisc	0.0005736	Pa×s	456.28	Joback Method
dvisc	0.0003806	Pa×s	499.69	Joback Method
dvisc	0.0002697	Pa×s	543.09	Joback Method
dvisc	0.0002011	Pa×s	586.50	Joback Method
dvisc	0.0001561	Pa×s	629.90	Joback Method

Sources

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=C581555&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chs: Standard solid enthalpy of combustion
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfs: Solid phase enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hsub: Enthalpy of sublimation 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