Benzeneethanol, «alpha»,«alpha»-dimethyl-, acetate

Other names: Phenethyl alcohol, «alpha»,«alpha»-dimethyl-, acetate
«alpha»,«alpha»-Dimethylphenethyl acetate
Benzyldimethylcarbinol acetate
Dimethylbenzylcarbinol acetate
Dimethylbenzylcarbinyl acetate
DMBCA
Acetic acid «alpha»,«alpha»-dimethyl-«beta»-phenylethyl ester
«alpha»,«alpha»-Dimethylphenethyl alcohol, acetate
Benzyldimethylcarbinyl acetate
2-Methyl-1-phenyl-2-propyl acetate
Benzeneethanol, «alpha»,«alpha»-dimethyl-, 1-acetate
NSC 46123

Inchi: InChI=1S/C12H16O2/c1-10(13)14-12(2,3)9-11-7-5-4-6-8-11/h4-8H,9H2,1-3H3

InchiKey: FLUWAIIVLCVEKF-UHFFFAOYSA-N

Formula: C12H16O2

SMILES: CC(=O)OC(C)(C)Cc1ccccc1

Mol. weight [g/mol]: 192.25

CAS: 151-05-3

Physical Properties

Property code	Value	Unit	Source
gf	-68.51	kJ/mol	Joback Method
hf	-308.03	kJ/mol	Joback Method
hfus	16.25	kJ/mol	Joback Method
hvap	52.44	kJ/mol	Joback Method
log10ws	-2.92		Crippen Method
logp	2.571		Crippen Method
mcvol	163.620	ml/mol	McGowan Method
pc	2566.29	kPa	Joback Method
rinpol	1297.50		NIST Webbook
tb	573.70	K	Joback Method
tc	792.31	K	Joback Method
tf	326.00	K	Joback Method
vc	0.613	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	397.32	J/mol×K	573.70	Joback Method
cpg	413.41	J/mol×K	610.13	Joback Method
cpg	428.45	J/mol×K	646.57	Joback Method
cpg	442.47	J/mol×K	683.00	Joback Method
cpg	455.52	J/mol×K	719.44	Joback Method
cpg	467.66	J/mol×K	755.87	Joback Method
cpg	478.93	J/mol×K	792.31	Joback Method
dvisc	0.0026378	Pa×s	326.00	Joback Method
dvisc	0.0012864	Pa×s	367.28	Joback Method
dvisc	0.0007254	Pa×s	408.57	Joback Method
dvisc	0.0004544	Pa×s	449.85	Joback Method
dvisc	0.0003079	Pa×s	491.13	Joback Method
dvisc	0.0002216	Pa×s	532.42	Joback Method
dvisc	0.0001672	Pa×s	573.70	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C151053&Units=SI

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