Benzenemethanol, «alpha»,«alpha»-dimethyl-, acetate

Other names: Acetic acid, 2-phenyl-2-propyl ester
1-methyl-1-phenylethyl acetate
2-Propanol, 2-phenyl, acetate

Inchi: InChI=1S/C11H14O2/c1-9(12)13-11(2,3)10-7-5-4-6-8-10/h4-8H,1-3H3

InchiKey: XPMMKIYJJWQFOR-UHFFFAOYSA-N

Formula: C11H14O2

SMILES: CC(=O)OC(C)(C)c1ccccc1

Mol. weight [g/mol]: 178.23

CAS: 3425-72-7

Physical Properties

Property code	Value	Unit	Source
gf	-76.93	kJ/mol	Joback Method
hf	-287.39	kJ/mol	Joback Method
hfus	13.66	kJ/mol	Joback Method
hvap	50.22	kJ/mol	Joback Method
log10ws	-2.56		Crippen Method
logp	2.485		Crippen Method
mcvol	149.530	ml/mol	McGowan Method
pc	2835.36	kPa	Joback Method
rinpol	1302.00		NIST Webbook
ripol	1755.00		NIST Webbook
tb	550.82	K	Joback Method
tc	773.39	K	Joback Method
tf	314.73	K	Joback Method
vc	0.556	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	349.74	J/mol×K	550.82	Joback Method
cpg	365.17	J/mol×K	587.91	Joback Method
cpg	379.55	J/mol×K	625.01	Joback Method
cpg	392.95	J/mol×K	662.10	Joback Method

cpg	405.40	J/mol×K	699.20	Joback Method
cpg	416.95	J/mol×K	736.29	Joback Method
cpg	427.65	J/mol×K	773.39	Joback Method
dvisc	0.0027809	Pa×s	314.73	Joback Method
dvisc	0.0013780	Pa×s	354.08	Joback Method
dvisc	0.0007858	Pa×s	393.43	Joback Method
dvisc	0.0004963	Pa×s	432.77	Joback Method
dvisc	0.0003384	Pa×s	472.12	Joback Method
dvisc	0.0002448	Pa×s	511.47	Joback Method
dvisc	0.0001854	Pa×s	550.82	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3425727&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume