

Benzenemethanol, «alpha»-methyl-, acetate

Other names:	Benzyol alcohol, «alpha»-methyl-, acetate «alpha»-Methylbenzyl acetate «alpha»-Phenylethyl acetate sec-Phenylethyl acetate Gardeniol II Gardenol Methylphenylcarbinol acetate Methylphenylcarbinyol acetate Styralyl acetate 1-Phenylethyl acetate Phenylmethylcarbinyol acetate Styrallyl acetate 1-Acetoxy-1-phenylethane NSC 2397 Styrylallyl acetate «alpha»-Methylbenzyl alcohol, acetate Acetic acid, 1-phenylethyl ester .+/--«alpha»-Methylbenzyl acetate
Inchi:	InChI=1S/C10H12O2/c1-8(12-9(2)11)10-6-4-3-5-7-10/h3-8H,1-2H3
InchiKey:	QUMXDOLUJCHOAY-UHFFFAOYSA-N
Formula:	C10H12O2
SMILES:	CC(=O)OC(C)c1ccccc1
Mol. weight [g/mol]:	164.20
CAS:	50373-55-2

Physical Properties

Property code	Value	Unit	Source
gf	-90.63	kJ/mol	Joback Method
hf	-263.28	kJ/mol	Joback Method
hfus	14.96	kJ/mol	Joback Method
hvap	48.90	kJ/mol	Joback Method
log10ws	-2.43		Crippen Method
logp	2.311		Crippen Method
mccvol	135.440	ml/mol	McGowan Method
pc	3110.57	kPa	Joback Method
tb	530.73	K	Joback Method
tc	748.19	K	Joback Method

tf	286.04	K	Joback Method
vc	0.505	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	300.78	J/mol×K	530.73	Joback Method
cpg	314.76	J/mol×K	566.97	Joback Method
cpg	327.92	J/mol×K	603.22	Joback Method
cpg	340.30	J/mol×K	639.46	Joback Method
cpg	351.91	J/mol×K	675.70	Joback Method
cpg	362.77	J/mol×K	711.95	Joback Method
cpg	372.90	J/mol×K	748.19	Joback Method
dvisc	0.0031130	Paxs	286.04	Joback Method
dvisc	0.0014883	Paxs	326.82	Joback Method
dvisc	0.0008382	Paxs	367.60	Joback Method
dvisc	0.0005294	Paxs	408.38	Joback Method
dvisc	0.0003634	Paxs	449.17	Joback Method
dvisc	0.0002656	Paxs	489.95	Joback Method
dvisc	0.0002037	Paxs	530.73	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	367.70	K	1.60	NIST Webbook

Sources

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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=C50373552&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
hvac:	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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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