3-Methylbenzyl acetate

Other names:	m-Methylbenzyl acetate
	Benzenemethanol, 3-methyl-, acetate
	Acetic acid, (3-methylphenyl)methyl ester
Inchi:	InChI=1S/C10H12O2/c1-8-4-3-5-10(6-8)7-12-9(2)11/h3-6H,7H2,1-2H3
InchiKey:	QPTQLFCBVFKFLY-UHFFFAOYSA-N
Formula:	C10H12O2
SMILES:	CC(=O)OCc1cccc(C)c1
Mol. weight [g/mol]:	164.20
CAS:	17369-57-2

Physical Properties

Property code	Value	Unit	Source
gf	-97.82	kJ/mol	Joback Method
hf	-269.47	kJ/mol	Joback Method
hfus	18.10	kJ/mol	Joback Method
hvap	49.95	kJ/mol	Joback Method
log10ws	-2.53		Crippen Method
logp	2.058		Crippen Method
mcvol	135.440	ml/mol	McGowan Method
pc	3032.27	kPa	Joback Method
rinpol	1283.00		NIST Webbook
rinpol	1283.00		NIST Webbook
tb	536.15	K	Joback Method
tc	749.95	K	Joback Method
tf	313.56	K	Joback Method
vc	0.511	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	300.27	J/mol×K	536.15	Joback Method
cpg	313.54	J/mol×K	571.78	Joback Method
cpg	326.10	J/mol×K	607.42	Joback Method
cpg	337.97	J/mol×K	643.05	Joback Method

cpg	349.15	J/mol×K	678.68	Joback Method
cpg	359.66	J/mol×K	714.31	Joback Method
cpg	369.52	J/mol×K	749.95	Joback Method
dvisc	0.0017515	Pa×s	313.56	Joback Method
dvisc	0.0010200	Pa×s	350.66	Joback Method
dvisc	0.0006587	Pa×s	387.76	Joback Method
dvisc	0.0004592	Pa×s	424.86	Joback Method
dvisc	0.0003392	Pa×s	461.95	Joback Method
dvisc	0.0002621	Pa×s	499.05	Joback Method
dvisc	0.0002099	Pa×s	536.15	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C17369572&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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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