

p-Methylbenzyl acetate

Other names:	4-Methylbenzyl acetate Benzenemethanol, 4-methyl-, acetate p-Tolubenzyl acetate p-Xylene, «alpha»-acetoxo p-Xylyl acetate Benzyl alcohol, p-methyl-, acetate 4-Methylbenzyl ethanoate Benzenemethanol, 4-methyl-, 1-acetate NSC 7001 p-Acetoxymethyltoluene Acetic acid, (4-methylphenyl)methyl ester
Inchi:	InChI=1S/C10H12O2/c1-8-3-5-10(6-4-8)7-12-9(2)11/h3-6H,7H2,1-2H3
InchiKey:	WDCUPFMSLUIQBH-UHFFFAOYSA-N
Formula:	C10H12O2
SMILES:	<chem>CC(=O)OCc1ccc(C)cc1</chem>
Mol. weight [g/mol]:	164.20
CAS:	2216-45-7

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
mvol	135.440	ml/mol	McGowan Method
pc	3032.27	kPa	Joback Method
rinpol	1290.00		NIST Webbook
tb	536.15	K	Joback Method
tc	749.95	K	Joback Method
tf	313.56	K	Joback Method
vc	0.511	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	300.27	J/molxK	536.15	Joback Method
cpg	313.54	J/molxK	571.78	Joback Method
cpg	326.10	J/molxK	607.42	Joback Method
cpg	337.97	J/molxK	643.05	Joback Method
cpg	349.15	J/molxK	678.68	Joback Method
cpg	359.66	J/molxK	714.31	Joback Method
cpg	369.52	J/molxK	749.95	Joback Method
dvisc	0.0017515	Paxs	313.56	Joback Method
dvisc	0.0010200	Paxs	350.66	Joback Method
dvisc	0.0006587	Paxs	387.76	Joback Method
dvisc	0.0004592	Paxs	424.86	Joback Method
dvisc	0.0003392	Paxs	461.95	Joback Method
dvisc	0.0002621	Paxs	499.05	Joback Method
dvisc	0.0002099	Paxs	536.15	Joback Method

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=C2216457&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

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