4-METHYLBENZYL ACETATE

Other names:	4-Methylbenzyl acetate
	Benzenemethanol, 4-methyl-, acetate
	p-Tolubenzyl acetate
	p-Xylene, «alpha»-acetoxy
	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:	CC(=O)OCc1ccc(C)cc1
Mol. weight [g/mol]:	164.20

Physical Properties

Property code	Value	Unit	Source
af	0.5004		Cheméo Relay (1.0)
gf	-97.82	kJ/mol	Joback Method
hf	-327.40	kJ/mol	Cheméo Relay (1.0)
hfus	18.10	kJ/mol	Joback Method
hvap	61.36	kJ/mol	Cheméo Relay (1.0)
ie	8.54	eV	Cheméo Relay (1.0)
log10ws	-2.35		Cheméo Relay (1.0)
logp	2.058		Crippen Method
mcvol	135.440	ml/mol	McGowan Method
pc	3032.27	kPa	Joback Method
rinpol	1290.00		NIST Webbook
tb	493.42	K	Cheméo Relay (1.0)
tc	705.95	K	Cheméo Relay (1.0)
tf	259.18	K	Cheméo Relay (1.0)
vc	0.502	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

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

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2216457&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af: Acentric Factor
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
ie:	Ionization energy
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