Benzenemethanol, 4-methoxy-, acetate

Other names:	Benzyl alcohol, p-methoxy-, acetate
	p-Methoxybenzyl acetate
	p-Methoxybenzyl alcohol acetate
	Cassie ketone
	4-Methoxybenzyl acetate
	p-Anisyl acetate
	Acetic acid p-methoxybenzyl ester
	4-Anisyl acetate
	Benzenemethanol, 4-methoxy-, 1-acetate
	NSC 46102
Inchi:	InChI=1S/C10H12O3/c1-8(11)13-7-9-3-5-10(12-2)6-4-9/h3-6H,7H2,1-2H3
InchiKey:	HFNGYHHRRMSKEU-UHFFFAOYSA-N
Formula:	C10H12O3
SMILES:	COc1ccc(COC(C)=O)cc1
Mol. weight [g/mol]:	180.20
CAS:	104-21-2

Physical Properties

Property code	Value	Unit	Source
gf	-202.82	kJ/mol	Joback Method
hf	-401.69	kJ/mol	Joback Method
hfus	19.28	kJ/mol	Joback Method
hvap	52.36	kJ/mol	Joback Method
log10ws	-2.17		Crippen Method
logp	1.758		Crippen Method
mcvol	141.310	ml/mol	McGowan Method
pc	2976.29	kPa	Joback Method
tb	558.57	K	Joback Method
tc	770.06	K	Joback Method
tf	335.79	K	Joback Method
vc	0.529	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	323.98	J/mol×K	558.57	Joback Method
cpg	382.66	J/mol×K	734.81	Joback Method
cpg	372.24	J/mol×K	699.56	Joback Method
cpg	361.16	J/mol×K	664.31	Joback Method
cpg	349.42	J/mol×K	629.07	Joback Method
cpg	337.02	J/mol×K	593.82	Joback Method
cpg	392.43	J/mol×K	770.06	Joback Method
dvisc	0.0001728	Pa×s	558.57	Joback Method
dvisc	0.0002153	Pa×s	521.44	Joback Method
dvisc	0.0002774	Pa×s	484.31	Joback Method
dvisc	0.0003728	Pa×s	447.18	Joback Method
dvisc	0.0005287	Pa×s	410.05	Joback Method
dvisc	0.0008036	Pa×s	372.92	Joback Method
dvisc	0.0013400	Pa×s	335.79	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	410.00	K	1.60	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C104212&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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume