O-ACETOXYBENZOYL CHLORIDE

Other names:	o-Acetylsalicyloyl chloride
	Acetylsalicoyl chloride
	o-Acetylsalicoyl chloride
	Benzoyl chloride, 2-(acetyloxy)-
	2-acetoxybenzoyl chloride
Inchi:	InChI=1S/C9H7ClO3/c1-6(11)13-8-5-3-2-4-7(8)9(10)12/h2-5H,1H3
InchiKey:	DSGKWFGEUBCEIE-UHFFFAOYSA-N
Formula:	C9H7ClO3
SMILES:	CC(=O)Oc1ccccc1C(=O)Cl
Mol. weight [g/mol]:	198.61

Physical Properties

Property code	Value	Unit	Source
hf	-468.87	kJ/mol	Cheméo Relay (1.0)
hfus	21.30	kJ/mol	Joback Method
hvap	69.37	kJ/mol	Cheméo Relay (1.0)
ie	8.95	eV	Cheméo Relay (1.0)
log10ws	-2.59		Cheméo Relay (1.0)
logp	1.991		Crippen Method
mcvol	135.160	ml/mol	McGowan Method
tb	527.85	K	Cheméo Relay (1.0)
tf	275.77	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	292.64	J/mol×K	604.57	Joback Method
cpg	344.26	J/mol×K	834.38	Joback Method
cpg	337.33	J/mol×K	796.08	Joback Method
cpg	329.75	J/mol×K	757.78	Joback Method
cpg	321.51	J/mol×K	719.48	Joback Method
cpg	312.58	J/mol×K	681.17	Joback Method
cpg	302.96	J/mol×K	642.87	Joback Method
dvisc	0.0004954	Pa×s	493.36	Joback Method

dvisc	0.0002416	Pa×s	604.57	Joback Method
dvisc	0.0002975	Pa×s	567.50	Joback Method
dvisc	0.0003771	Pa×s	530.43	Joback Method
dvisc	0.0015429	Pa×s	382.14	Joback Method
dvisc	0.0006803	Pa×s	456.28	Joback Method
dvisc	0.0009881	Pa×s	419.21	Joback Method

Sources

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
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=C5538512&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point