

3,4-Dimethoxybenzoyl chloride

Other names:	Benzoyl chloride, 3,4-dimethoxy-veratroyl chloride
Inchi:	InChI=1S/C9H9ClO3/c1-12-7-4-3-6(9(10)11)5-8(7)13-2/h3-5H,1-2H3
InchiKey:	VIOBGCWEHLRBEP-UHFFFAOYSA-N
Formula:	C9H9ClO3
SMILES:	COc1ccc(C(=O)Cl)cc1OC
Mol. weight [g/mol]:	200.62
CAS:	3535-37-3

Physical Properties

Property code	Value	Unit	Source
gf	-232.80	kJ/mol	Joback Method
hf	-408.26	kJ/mol	Joback Method
hfus	20.50	kJ/mol	Joback Method
hvap	55.18	kJ/mol	Joback Method
log10ws	-2.60		Crippen Method
logp	2.083		Crippen Method
mvol	139.460	ml/mol	McGowan Method
pc	3124.49	kPa	Joback Method
rinpol	1606.90		NIST Webbook
tb	578.10	K	Joback Method
tc	798.52	K	Joback Method
tf	366.96	K	Joback Method
vc	0.522	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	302.40	J/molxK	578.10	Joback Method
cpg	313.52	J/molxK	614.84	Joback Method
cpg	324.06	J/molxK	651.57	Joback Method
cpg	334.01	J/molxK	688.31	Joback Method
cpg	343.37	J/molxK	725.05	Joback Method
cpg	352.12	J/molxK	761.78	Joback Method

cpg	360.25	J/mol×K	798.52	Joback Method
dvisc	0.0010339	Paxs	366.96	Joback Method
dvisc	0.0006811	Paxs	402.15	Joback Method
dvisc	0.0004798	Paxs	437.34	Joback Method
dvisc	0.0003562	Paxs	472.53	Joback Method
dvisc	0.0002755	Paxs	507.72	Joback Method
dvisc	0.0002203	Paxs	542.91	Joback Method
dvisc	0.0001811	Paxs	578.10	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3535373&Units=SI
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

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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