3,5-DIMETHOXYBENZOYL CHLORIDE

Other names: Benzoyl chloride, 3,5-dimethoxy-
Inchi: InChI=1S/C9H9ClO3/c1-12-7-3-6(9(10)11)4-8(5-7)13-2/h3-5H,1-2H3
InchiKey: FTHPLWDYWAKYCY-UHFFFAOYSA-N
Formula: C9H9ClO3
SMILES: COc1cc(OC)cc(C(=O)Cl)c1
Mol. weight [g/mol]: 200.62

Physical Properties

Property code	Value	Unit	Source
hf	-402.99	kJ/mol	Cheméo Relay (1.0)
hfus	20.50	kJ/mol	Joback Method
hvap	75.13	kJ/mol	Cheméo Relay (1.0)
ie	8.55	eV	Cheméo Relay (1.0)
log10ws	-3.36		Cheméo Relay (1.0)
logp	2.083		Crippen Method
mcvol	139.460	ml/mol	McGowan Method
tb	546.33	K	Cheméo Relay (1.0)
tf	319.70	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	302.40	J/mol×K	578.10	Joback Method
cpg	360.25	J/mol×K	798.52	Joback Method
cpg	352.12	J/mol×K	761.78	Joback Method
cpg	343.37	J/mol×K	725.05	Joback Method
cpg	334.01	J/mol×K	688.31	Joback Method
cpg	324.06	J/mol×K	651.57	Joback Method
cpg	313.52	J/mol×K	614.84	Joback Method
dvisc	0.0003562	Pa×s	472.53	Joback Method
dvisc	0.0001811	Pa×s	578.10	Joback Method
dvisc	0.0002203	Pa×s	542.91	Joback Method
dvisc	0.0002755	Pa×s	507.72	Joback Method
dvisc	0.0010339	Pa×s	366.96	Joback Method

dvisc	0.0004798	Pa×s	437.34	Joback Method
dvisc	0.0006811	Pa×s	402.15	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	430.70	K	2.10	NIST Webbook

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C17213579&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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

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
tbrp: Boiling point at reduced pressure
tf: Normal melting (fusion) point