3,4,5-Trimethoxybenzyl chloride

Other names: Benzene, 5-(chloromethyl)-1,2,3-trimethoxy-
5-(chloromethyl)-1,2,3-trimethoxybenzene
Inchi: InChI=1S/C10H13ClO3/c1-12-8-4-7(6-11)5-9(13-2)10(8)14-3/h4-5H,6H2,1-3H3
InchiKey: XXRUQNNAKXZSOS-UHFFFAOYSA-N
Formula: C10H13ClO3
SMILES: COc1cc(CCl)cc(OC)c1OC
Mol. weight [g/mol]: 216.66
CAS: 3840-30-0

Physical Properties

Property code	Value	Unit	Source
gf	-210.09	kJ/mol	Joback Method
hf	-460.01	kJ/mol	Joback Method
hfus	22.29	kJ/mol	Joback Method
hvap	53.73	kJ/mol	Joback Method
log10ws	-2.86		Crippen Method
logp	2.451		Crippen Method
mcvol	157.850	ml/mol	McGowan Method
pc	2550.76	kPa	Joback Method
tb	574.51	K	Joback Method
tc	782.12	K	Joback Method
tf	363.05	K	Joback Method
vc	0.591	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	356.49	J/mol×K	574.51	Joback Method
cpg	369.20	J/mol×K	609.11	Joback Method
cpg	381.40	J/mol×K	643.71	Joback Method
cpg	393.06	J/mol×K	678.32	Joback Method
cpg	404.15	J/mol×K	712.92	Joback Method
cpg	414.66	J/mol×K	747.52	Joback Method
cpg	424.56	J/mol×K	782.12	Joback Method

dvisc	0.0006690	Pa×s	363.05	Joback Method
dvisc	0.0004454	Pa×s	398.29	Joback Method
dvisc	0.0003168	Pa×s	433.54	Joback Method
dvisc	0.0002372	Pa×s	468.78	Joback Method
dvisc	0.0001849	Pa×s	504.02	Joback Method
dvisc	0.0001489	Pa×s	539.27	Joback Method
dvisc	0.0001232	Pa×s	574.51	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3840300&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume