3,4-Methylenedioxybenzyl chloride

Other names:	1,3-Benzodioxole, 5-(chloromethyl)-
	Piperonyl chloride
	Toluene, «alpha»-chloro-3,4-(methylenedioxy)-
	4-Chloromethyl-1,2-methylenedioxybenzene
	5-(Chloromethyl)-1,3-benzodioxole
	5-chloro-1,3-benzodioxole
Inchi:	InChI=1S/C8H7ClO2/c9-4-6-1-2-7-8(3-6)11-5-10-7/h1-3H,4-5H2
InchiKey:	DWSUJONSJJTODA-UHFFFAOYSA-N
Formula:	C8H7ClO2
SMILES:	ClCc1ccc2c(c1)OCO2
Mol. weight [g/mol]:	170.59
CAS:	20850-43-5

Physical Properties

Property code	Value	Unit	Source
gf	-6.08	kJ/mol	Joback Method
hf	-181.46	kJ/mol	Joback Method
hfus	26.96	kJ/mol	Joback Method
hvap	50.63	kJ/mol	Joback Method
log10ws	-2.71		Crippen Method
logp	2.154		Crippen Method
mcvol	112.940	ml/mol	McGowan Method
pc	4021.02	kPa	Joback Method
rinpol	1300.00		NIST Webbook
rinpol	1300.00		NIST Webbook
rinpol	1300.00		NIST Webbook
tb	521.82	K	Joback Method
tc	756.18	K	Joback Method
tf	336.62	K	Joback Method
vc	0.424	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	238.31	J/mol×K	521.82	Joback Method
cpg	284.63	J/mol×K	717.12	Joback Method
cpg	276.79	J/mol×K	678.06	Joback Method
cpg	268.31	J/mol×K	639.00	Joback Method
cpg	259.11	J/mol×K	599.94	Joback Method
cpg	249.13	J/mol×K	560.88	Joback Method
cpg	291.87	J/mol×K	756.18	Joback Method
dvisc	0.0005210	Pa×s	521.82	Joback Method
dvisc	0.0006132	Pa×s	490.95	Joback Method
dvisc	0.0007376	Pa×s	460.09	Joback Method
dvisc	0.0009111	Pa×s	429.22	Joback Method
dvisc	0.0011628	Pa×s	398.35	Joback Method
dvisc	0.0015462	Pa×s	367.49	Joback Method
dvisc	0.0021664	Pa×s	336.62	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=C20850435&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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume