3-CHLOROPERBENZOIC ACID

Other names:	m-Chloroperbenzoic acid
	Benzenecarboperoxoic acid, 3-chloro-
	m-Chlorobenzoyl hydroperoxide
	m-Chloroperoxybenzoic acid
	Perbenzoic acid, m-chloro-
	Peroxybenzoic acid, m-chloro-
	3-Chloroperoxybenzoic acid
	UN 2755
	MCPBA
	NSC 97094
Inchi:	InChI=1S/C7H5ClO3/c8-6-3-1-2-5(4-6)7(9)11-10/h1-4,10H
InchiKey:	NHQDETIJWKXCTC-UHFFFAOYSA-N
Formula:	C7H5ClO3
SMILES:	O=C(OO)c1cccc(Cl)c1
Mol. weight [g/mol]:	172.57

Physical Properties

Property code	Value	Unit	Source
hf	-272.75	kJ/mol	Cheméo Relay (1.0)
hfus	18.61	kJ/mol	Joback Method
hvap	82.00	kJ/mol	Cheméo Relay (1.0)
ie	9.90	eV	Cheméo Relay (1.0)
log10ws	-2.48		Cheméo Relay (1.0)
logp	1.970		Crippen Method
mcvol	111.280	ml/mol	McGowan Method
pc	4608.87	kPa	Joback Method
tb	518.82	K	Cheméo Relay (1.0)
tc	781.89	K	Cheméo Relay (1.0)
tf	320.16	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	234.09	J/mol×K	597.12	Joback Method

cpg	241.65	J/mol×K	632.55	Joback Method
cpg	248.74	J/mol×K	667.98	Joback Method
cpg	255.36	J/mol×K	703.41	Joback Method
cpg	261.51	J/mol×K	738.85	Joback Method
cpg	267.22	J/mol×K	774.28	Joback Method
cpg	272.47	J/mol×K	809.71	Joback Method
dvisc	0.0025401	Pa×s	370.49	Joback Method
dvisc	0.0011393	Pa×s	408.26	Joback Method
dvisc	0.0005853	Pa×s	446.03	Joback Method
dvisc	0.0003336	Pa×s	483.81	Joback Method
dvisc	0.0002063	Pa×s	521.58	Joback Method
dvisc	0.0001361	Pa×s	559.35	Joback Method
dvisc	0.0000947	Pa×s	597.12	Joback Method

Sources

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=C937144&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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
pc: Critical Pressure
tb: Normal Boiling Point Temperature
tc: Critical Temperature

tf: Normal melting (fusion) point