

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
CAS:	937-14-4

Physical Properties

Property code	Value	Unit	Source
gf	-271.83	kJ/mol	Joback Method
hf	-375.52	kJ/mol	Joback Method
hfus	18.61	kJ/mol	Joback Method
hvap	64.33	kJ/mol	Joback Method
log10ws	-2.29		Crippen Method
logp	1.970		Crippen Method
mcvol	111.280	ml/mol	McGowan Method
pc	4608.87	kPa	Joback Method
tb	597.12	K	Joback Method
tc	809.71	K	Joback Method
tf	370.49	K	Joback Method
vc	0.411	m3/kmol	Joback Method

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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C937144&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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

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

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