

Benzoic acid, 2,4,6-trichloro-

Other names:	2,4,6-Trichlorobenzoic acid
Inchi:	InChI=1S/C7H3Cl3O2/c8-3-1-4(9)6(7(11)12)5(10)2-3/h1-2H,(H,11,12)
InchiKey:	RAFFVQBMVYYTQS-UHFFFAOYSA-N
Formula:	C7H3Cl3O2
SMILES:	O=C(O)c1c(Cl)cc(Cl)cc1Cl
Mol. weight [g/mol]:	225.46
CAS:	50-43-1

Physical Properties

Property code	Value	Unit	Source
gf	-209.95	kJ/mol	Joback Method
hf	-297.72	kJ/mol	Joback Method
hfus	25.04	kJ/mol	Joback Method
hvap	72.02	kJ/mol	Joback Method
log10ws	-3.59		Crippen Method
logp	3.345		Crippen Method
mcvol	129.890	ml/mol	McGowan Method
pc	4109.14	kPa	Joback Method
tb	659.52	K	Joback Method
tc	883.58	K	Joback Method
tf	433.14	K	Joback Method
vc	0.491	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	247.03	J/mol×K	659.52	Joback Method
cpg	271.85	J/mol×K	846.23	Joback Method
cpg	267.68	J/mol×K	808.89	Joback Method
cpg	263.13	J/mol×K	771.55	Joback Method
cpg	258.18	J/mol×K	734.21	Joback Method
cpg	252.82	J/mol×K	696.86	Joback Method
cpg	275.65	J/mol×K	883.58	Joback Method
dvisc	0.0000877	Paxs	659.52	Joback Method

dvisc	0.0001192	Paxs	621.79	Joback Method
dvisc	0.0001684	Paxs	584.06	Joback Method
dvisc	0.0002496	Paxs	546.33	Joback Method
dvisc	0.0003923	Paxs	508.60	Joback Method
dvisc	0.0006628	Paxs	470.87	Joback Method
dvisc	0.0012269	Paxs	433.14	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C50431&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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