Benzoic acid, 2,3,6-trichloro-

Other names:	Benzac 1,281
	HC 1281
	T-2
	Trysben
	TCB
	2,3,6-Trichlorobenzoic acid
	2,3,6-TBA
	2,3,6-TCBA
	Acide trichlorobenzoique
	Benzabar
	Benzac-1281
	Benzak
	Fen-all
	Kyselina 2,3,6-trichlorbenzoova
	NCI-C60242
	2,3,6-Tba(the herbicide)
	2,3,6-TCB
	TCBA
	Tribac
	2,3,6-Trichlorbenzoesaeure
	Trichlorobenzoic acid
	Trisben
Inchi:	InChI=1S/C7H3Cl3O2/c8-3-1-2-4(9)6(10)5(3)7(11)12/h1-2H,(H,11,12)
InchiKey:	XZIDTOHMJBOSOX-UHFFFAOYSA-N
Formula:	C7H3Cl3O2
SMILES:	O=C(O)c1c(Cl)ccc(Cl)c1Cl
Mol. weight [g/mol]:	225.46
CAS:	50-31-7

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	402.70 ± 0.20	K	NIST Webbook
vc	0.491	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	271.85	J/mol×K	846.23	Joback Method
cpg	275.65	J/mol×K	883.58	Joback Method
cpg	247.03	J/mol×K	659.52	Joback Method
cpg	252.82	J/mol×K	696.86	Joback Method
cpg	258.18	J/mol×K	734.21	Joback Method
cpg	263.13	J/mol×K	771.55	Joback Method
cpg	267.68	J/mol×K	808.89	Joback Method
dvisc	0.0000877	Pa×s	659.52	Joback Method
dvisc	0.0001192	Pa×s	621.79	Joback Method
dvisc	0.0012269	Pa×s	433.14	Joback Method
dvisc	0.0006628	Pa×s	470.87	Joback Method
dvisc	0.0003923	Pa×s	508.60	Joback Method
dvisc	0.0002496	Pa×s	546.33	Joback Method
dvisc	0.0001684	Pa×s	584.06	Joback Method
hfust	23.85	kJ/mol	402.70	NIST Webbook
hfust	23.85	kJ/mol	402.70	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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=C50317&Units=SI

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
hfust:	Enthalpy of fusion at a given temperature
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