3,5-Dichlorobenzoic acid

Other names: Benzoic acid, 3,5-dichloro-
Inchi: InChI=1S/C7H4Cl2O2/c8-5-1-4(7(10)11)2-6(9)3-5/h1-3H,(H,10,11)
InchiKey: CXKCZFDUOYMOOP-UHFFFAOYSA-N
Formula: C7H4Cl2O2
SMILES: O=C(O)c1cc(Cl)cc(Cl)c1
Mol. weight [g/mol]: 191.01
CAS: 51-36-5

Physical Properties

Property code	Value	Unit	Source
gf	-188.39	kJ/mol	Joback Method
hf	-270.51	kJ/mol	Joback Method
hfus	21.23	kJ/mol	Joback Method
hvap	66.97	kJ/mol	Joback Method
log10ws	-2.90		Crippen Method
logp	2.692		Crippen Method
mcvol	117.650	ml/mol	McGowan Method
pc	4397.41	kPa	Joback Method
tb	617.11	K	Joback Method
tc	836.94	K	Joback Method
tf	460.51 ± 0.20	K	NIST Webbook
vc	0.443	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	231.22	J/mol×K	617.11	Joback Method
cpg	237.87	J/mol×K	653.75	Joback Method
cpg	244.04	J/mol×K	690.39	Joback Method
cpg	249.76	J/mol×K	727.03	Joback Method
cpg	255.05	J/mol×K	763.66	Joback Method
cpg	259.93	J/mol×K	800.30	Joback Method
cpg	264.41	J/mol×K	836.94	Joback Method
dvisc	0.0021517	Pa×s	390.70	Joback Method

dvisc	0.0010438	Pa×s	428.44	Joback Method
dvisc	0.0005693	Pa×s	466.17	Joback Method
dvisc	0.0003400	Pa×s	503.90	Joback Method
dvisc	0.0002182	Pa×s	541.64	Joback Method
dvisc	0.0001483	Pa×s	579.38	Joback Method
dvisc	0.0001057	Pa×s	617.11	Joback Method
hfust	22.97	kJ/mol	459.30	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=C51365&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