2,4-Dichlorobenzyl mercaptan

Other names: Benzenemethanethiol, 3,4-dichloro-
3,4-dichlorotoluene-«alpha»-thiol
Inchi: InChI=1S/C7H6Cl2S/c8-6-2-1-5(4-10)3-7(6)9/h1-3,10H,4H2
InchiKey: CEGBRSQPRQXALB-UHFFFAOYSA-N
Formula: C7H6Cl2S
SMILES: SCc1ccc(Cl)c(Cl)c1
Mol. weight [g/mol]: 193.09
CAS: 36480-40-7

Physical Properties

Property code	Value	Unit	Source
gf	106.74	kJ/mol	Joback Method
hf	32.78	kJ/mol	Joback Method
hfus	19.59	kJ/mol	Joback Method
hvap	50.28	kJ/mol	Joback Method
log10ws	-3.79		Crippen Method
logp	3.423		Crippen Method
mcvol	126.560	ml/mol	McGowan Method
pc	3911.14	kPa	Joback Method
tb	533.92	K	Joback Method
tc	787.00	K	Joback Method
tf	316.41	K	Joback Method
vc	0.471	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	225.56	J/mol×K	533.92	Joback Method
cpg	235.08	J/mol×K	576.10	Joback Method
cpg	243.90	J/mol×K	618.28	Joback Method
cpg	252.07	J/mol×K	660.46	Joback Method
cpg	259.61	J/mol×K	702.64	Joback Method
cpg	266.56	J/mol×K	744.82	Joback Method
cpg	272.94	J/mol×K	787.00	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C36480407&Units=SI
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

Legend

cpg:	Ideal gas heat capacity
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