3,4-Dichlorobenzyl mercaptan

Other names:	3,4-dichlorotoluene-«alpha»-thiol
	Benzenemethanethiol, 3,4-dichloro-
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]:	193.10
CAS:	36480-40-7

Physical Properties

Property code	Value	Unit	Source
hf	-2.10	kJ/mol	Cheméo Relay (1.0)
hfus	19.59	kJ/mol	Joback Method
hvap	71.34	kJ/mol	Cheméo Relay (1.0)
ie	8.66	eV	Cheméo Relay (1.0)
log10ws	-3.35		Cheméo Relay (1.0)
logp	3.423		Crippen Method
mcvol	126.560	ml/mol	McGowan Method
tb	526.50	K	Cheméo Relay (1.0)
tf	281.37	K	Cheméo Relay (1.0)

Correlations

Information	Value
Property code	cpg
Equation	$Y = A + B \cdot T + C \cdot T^2 + D \cdot T^3 + E \cdot T.$
Y unit	J/mol×K
Coeff. A	3.18910e+01
Coeff. B	5.11800e-01
Coeff. C	-3.17320e-04
Coeff. D	7.14000e-08
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00

Temperature range (K), max.	1000.00

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C36480407&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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