2,6-Dichlorophenyl ethyl sulphide

Inchi: InChI=1S/C8H8Cl2S/c1-2-11-8-6(9)4-3-5-7(8)10/h3-5H,2H2,1H3
InchiKey: OCLSIUYYVUQKDI-UHFFFAOYSA-N
Formula: C8H8Cl2S
SMILES: CCSc1c(Cl)cccc1Cl
Mol. weight [g/mol]: 207.12
CAS: 207853-62-1

Physical Properties

Property code	Value	Unit	Source
gf	118.89	kJ/mol	Joback Method
hf	15.53	kJ/mol	Joback Method
hfus	22.26	kJ/mol	Joback Method
hvap	52.59	kJ/mol	Joback Method
log10ws	-4.00		Crippen Method
logp	4.105		Crippen Method
mcvol	140.650	ml/mol	McGowan Method
pc	3295.37	kPa	Joback Method
tb	562.72	K	Joback Method
tc	809.74	K	Joback Method
tf	325.62	K	Joback Method
vc	0.527	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	269.68	J/mol×K	562.72	Joback Method
cpg	280.57	J/mol×K	603.89	Joback Method
cpg	290.72	J/mol×K	645.06	Joback Method
cpg	300.15	J/mol×K	686.23	Joback Method
cpg	308.88	J/mol×K	727.40	Joback Method
cpg	316.93	J/mol×K	768.57	Joback Method
cpg	324.33	J/mol×K	809.74	Joback Method

Sources

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=C207853621&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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