2-Chloroethyl 4-chlorobutyl sulfide

Other names: Sulfide, 2-chloroethyl, 4-chlorobutyl
Inchi: InChI=1S/C6H12Cl2S/c7-3-1-2-5-9-6-4-8/h1-6H2
InchiKey: YVIBABWKOTUTDX-UHFFFAOYSA-N
Formula: C6H12Cl2S
SMILES: ClCCCCSCCCl
Mol. weight [g/mol]: 187.13

Physical Properties

Property code	Value	Unit	Source
gf	8.90	kJ/mol	Joback Method
hf	-156.78	kJ/mol	Joback Method
hfus	23.82	kJ/mol	Joback Method
hvap	44.54	kJ/mol	Joback Method
log10ws	-2.52		Crippen Method
logp	2.977		Crippen Method
mcvol	136.230	ml/mol	McGowan Method
pc	2918.68	kPa	Joback Method
rinpol	1312.30		NIST Webbook
rinpol	1269.00		NIST Webbook
rinpol	1312.30		NIST Webbook
rinpol	1269.00		NIST Webbook
tb	480.32	K	Joback Method
tc	682.49	K	Joback Method
tf	251.62	K	Joback Method
vc	0.523	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	257.92	J/mol×K	480.32	Joback Method
cpg	268.63	J/mol×K	514.02	Joback Method
cpg	278.83	J/mol×K	547.71	Joback Method
cpg	288.52	J/mol×K	581.41	Joback Method
cpg	297.74	J/mol×K	615.10	Joback Method

cpg	306.47	J/mol×K	648.80	Joback Method
cpg	314.74	J/mol×K	682.49	Joback Method

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=R41584&Units=SI

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume