Ethyl chloromethyl sulfide

Inchi: InChI=1S/C3H7ClS/c1-2-5-3-4/h2-3H2,1H3
InchiKey: XZCHJYXUPALGHH-UHFFFAOYSA-N
Formula: C3H7ClS
SMILES: CCSCCl
Mol. weight [g/mol]: 110.61

Physical Properties

Property code	Value	Unit	Source
gf	-4.43	kJ/mol	Joback Method
hf	-79.12	kJ/mol	Joback Method
hfus	11.85	kJ/mol	Joback Method
hvap	33.47	kJ/mol	Joback Method
log10ws	-1.61		Crippen Method
logp	1.936		Crippen Method
mcvol	81.720	ml/mol	McGowan Method
pc	4294.29	kPa	Joback Method
rinpol	822.00		NIST Webbook
tb	374.25	K	Joback Method
tc	575.61	K	Joback Method
tf	187.89	K	Joback Method
vc	0.306	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	124.75	J/mol×K	374.25	Joback Method
cpg	131.43	J/mol×K	407.81	Joback Method
cpg	137.86	J/mol×K	441.37	Joback Method
cpg	144.04	J/mol×K	474.93	Joback Method
cpg	149.97	J/mol×K	508.49	Joback Method
cpg	155.65	J/mol×K	542.05	Joback Method
cpg	161.08	J/mol×K	575.61	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R511665&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume