Sulfide, t-butyl-2-chloroethyl

Inchi: InChI=1S/C6H13ClS/c1-6(2,3)8-5-4-7/h4-5H2,1-3H3
InchiKey: FTZZXHJHQHXYRA-UHFFFAOYSA-N
Formula: C6H13ClS
SMILES: CC(C)(C)SCCCl
Mol. weight [g/mol]: 152.69
CAS: 4303-44-0

Physical Properties

Property code	Value	Unit	Source
gf	23.67	kJ/mol	Joback Method
hf	-149.79	kJ/mol	Joback Method
hfus	12.21	kJ/mol	Joback Method
hvap	38.86	kJ/mol	Joback Method
log10ws	-2.48		Crippen Method
logp	2.757		Crippen Method
mcvol	123.990	ml/mol	McGowan Method
pc	3103.64	kPa	Joback Method
tb	439.66	K	Joback Method
tc	648.99	K	Joback Method
tf	224.12	K	Joback Method
vc	0.464	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	235.36	J/mol×K	439.66	Joback Method
cpg	247.79	J/mol×K	474.55	Joback Method
cpg	259.52	J/mol×K	509.44	Joback Method
cpg	270.55	J/mol×K	544.32	Joback Method
cpg	280.94	J/mol×K	579.21	Joback Method
cpg	290.69	J/mol×K	614.10	Joback Method
cpg	299.85	J/mol×K	648.99	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=C4303440&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