2-Chloroethyl benzyl sulfide

Other names:	Benzyl 2-chloroethyl sulfide
	Benzene, [[(2-chloroethyl)thio]methyl]-
	Sulfide, benzyl 2-chloroethyl
	Benzyl «beta»-chloroethyl sulfide
	2-Benzylthioethyl chloride
	[[(2-chloroethyl)thio]methyl]benzene
Inchi:	InChI=1S/C9H11ClS/c10-6-7-11-8-9-4-2-1-3-5-9/h1-5H,6-8H2
InchiKey:	UQSMMTFBNJUPGW-UHFFFAOYSA-N
Formula:	C9H11ClS
SMILES:	ClCCSCc1ccccc1
Mol. weight [g/mol]:	186.70
CAS:	4332-51-8

Physical Properties

Property code	Value	Unit	Source
gf	158.50	kJ/mol	Joback Method
hf	33.57	kJ/mol	Joback Method
hfus	21.43	kJ/mol	Joback Method
hvap	49.11	kJ/mol	Joback Method
log10ws	-3.22		Crippen Method
logp	3.159		Crippen Method
mcvol	142.500	ml/mol	McGowan Method
pc	3188.33	kPa	Joback Method
tb	538.21	K	Joback Method
tc	773.70	K	Joback Method
tf	281.93	K	Joback Method
vc	0.534	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	350.28	J/mol×K	734.45	Joback Method
cpg	291.48	J/mol×K	538.21	Joback Method
cpg	305.01	J/mol×K	577.46	Joback Method

cpg	317.62	J/mol×K	616.71	Joback Method
cpg	329.34	J/mol×K	655.95	Joback Method
cpg	340.22	J/mol×K	695.20	Joback Method
cpg	359.58	J/mol×K	773.70	Joback Method
hvapt	52.30	kJ/mol	313.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4332518&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
hvapt:	Enthalpy of vaporization at a given temperature
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