Benzyl 2-chloroethyl sulfone

Other names: Benzene, [[(2-chloroethyl)sulfonyl]methyl]-
[[(2-chloroethyl)sulphonyl]methyl]benzene
Inchi: InChI=1S/C9H11ClO2S/c10-6-7-13(11,12)8-9-4-2-1-3-5-9/h1-5H,6-8H2
InchiKey: CKNUUVURUUCDGT-UHFFFAOYSA-N
Formula: C9H11ClO2S
SMILES: O=S(=O)(CCCl)Cc1ccccc1
Mol. weight [g/mol]: 218.70
CAS: 66998-67-2

Physical Properties

Property code	Value	Unit	Source
gf	-343.16	kJ/mol	Joback Method
hf	-461.65	kJ/mol	Joback Method
hfus	28.68	kJ/mol	Joback Method
hvap	60.92	kJ/mol	Joback Method
log10ws	-2.17		Crippen Method
logp	1.840		Crippen Method
mcvol	154.240	ml/mol	McGowan Method
pc	3749.97	kPa	Joback Method
tb	517.21	K	Joback Method
tc	723.65	K	Joback Method
tf	286.09	K	Joback Method
vc	0.607	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	319.63	J/mol×K	517.21	Joback Method
cpg	333.22	J/mol×K	551.62	Joback Method
cpg	346.01	J/mol×K	586.02	Joback Method
cpg	358.00	J/mol×K	620.43	Joback Method
cpg	369.22	J/mol×K	654.84	Joback Method
cpg	379.68	J/mol×K	689.24	Joback Method
cpg	389.41	J/mol×K	723.65	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=C66998672&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume