N,N-Bis(2-chloroethyl)-p-toluenesulfonamide

Other names: N,N-Bis(«beta»-chloroethyl)-p-toluenesulfonamide
Benzenesulfonamide, N,N-bis(2-chloroethyl)-4-methyl-
N,N-Bis-(2-chloro-ethyl)-4-methyl-benzenesulfonamide
N,N-bis(2-chloroethyl)-p-toluenesulphonamide
Inchi: InChI=1S/C11H15Cl2NO2S/c1-10-2-4-11(5-3-10)17(15,16)14(8-6-12)9-7-13/h2-5H,6-9H
InchiKey: PTVBBIMKLOMGSY-UHFFFAOYSA-N
Formula: C11H15Cl2NO2S
SMILES: Cc1ccc(S(=O)(=O)N(CCCl)CCCl)cc1
Mol. weight [g/mol]: 296.21
CAS: 42137-88-2

Physical Properties

Property code	Value	Unit	Source
gf	-237.10	kJ/mol	Joback Method
hf	-462.61	kJ/mol	Joback Method
hfus	40.69	kJ/mol	Joback Method
hvap	72.47	kJ/mol	Joback Method
log10ws	-2.76		Crippen Method
logp	2.463		Crippen Method
mcvol	204.640	ml/mol	McGowan Method
pc	2832.35	kPa	Joback Method
tb	617.82	K	Joback Method
tc	820.70	K	Joback Method
tf	383.54	K	Joback Method
vc	0.785	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	477.16	J/mol×K	617.82	Joback Method
cpg	491.44	J/mol×K	651.63	Joback Method
cpg	504.78	J/mol×K	685.45	Joback Method
cpg	517.22	J/mol×K	719.26	Joback Method
cpg	528.78	J/mol×K	753.07	Joback Method

cpg	539.49	J/mol×K	786.89	Joback Method
cpg	549.38	J/mol×K	820.70	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C42137882&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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