

Benzenesulfonamide, N,N'-(dithiodi-2,1-ethanediyl)bis[4-methyl-

Other names: p-Toluenesulfonamide, N,N'-(dithiodiethylene)bis-N,N'-Ditosylcystamine

Inchi: InChI=1S/C18H24N2O4S4/c1-15-3-7-17(8-4-15)27(21,22)19-11-13-25-26-14-12-20-28(2

InchiKey: FZPRKJHNYWETLJ-UHFFFAOYSA-N

Formula: C18H24N2O4S4

SMILES: Cc1ccc(S(=O)(=O)NCCSSCCNS(=O)(=O)c2ccc(C)cc2)cc1

Mol. weight [g/mol]: 460.65

CAS: 23516-74-7

Physical Properties

Property code	Value	Unit	Source
gf	-385.82	kJ/mol	Joback Method
hf	-680.75	kJ/mol	Joback Method
hfus	70.89	kJ/mol	Joback Method
hvap	125.31	kJ/mol	Joback Method
log10ws	-5.41		Crippen Method
logp	2.942		Crippen Method
mcvol	325.800	ml/mol	McGowan Method
pc	2646.11	kPa	Joback Method
tb	1008.02	K	Joback Method
tc	1247.05	K	Joback Method
tf	621.74	K	Joback Method
vc	1.258	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	972.12	J/molxK	1008.02	Joback Method
cpg	980.17	J/molxK	1047.86	Joback Method
cpg	986.21	J/molxK	1087.70	Joback Method
cpg	990.26	J/molxK	1127.53	Joback Method
cpg	992.33	J/molxK	1167.37	Joback Method
cpg	992.45	J/molxK	1207.21	Joback Method
cpg	990.63	J/molxK	1247.05	Joback Method

Sources

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=C23516747&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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