P-toluenesulfonamide, n-[2-(n-ethyl-p-toluenesulfonamido)ethyl]-n-(2-hyd

Inchi: InChI=1S/C20H28N2O5S2/c1-4-21(28(24,25)19-9-5-17(2)6-10-19)13-14-22(15-16-23)29

InchiKey: RXAPEZPIYSXMDK-UHFFFAOYSA-N

Formula: C20H28N2O5S2

SMILES: CCN(CCN(CCO)S(=O)(=O)c1ccc(C)cc1)S(=O)(=O)c1ccc(C)cc1

Mol. weight [g/mol]: 440.58

CAS: 23563-47-5

Physical Properties

Property code	Value	Unit	Source
gf	-529.26	kJ/mol	Joback Method
hf	-929.88	kJ/mol	Joback Method
hfus	67.75	kJ/mol	Joback Method
hvap	124.03	kJ/mol	Joback Method
log10ws	-3.52		Crippen Method
logp	1.997		Crippen Method
mcvol	327.150	ml/mol	McGowan Method
pc	2250.40	kPa	Joback Method
tb	932.94	K	Joback Method
tc	1143.80	K	Joback Method
tf	595.92	K	Joback Method
vc	1.246	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1018.47	J/mol×K	932.94	Joback Method
cpg	1031.03	J/mol×K	968.08	Joback Method
cpg	1042.17	J/mol×K	1003.23	Joback Method
cpg	1051.94	J/mol×K	1038.37	Joback Method
cpg	1060.37	J/mol×K	1073.51	Joback Method
cpg	1067.54	J/mol×K	1108.66	Joback Method
cpg	1073.47	J/mol×K	1143.80	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=C23563475&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