Perfluidone

Other names:	1,1,1-Trifluoro-4'-(phenylsulfonyl)methanesulfono-o-toluidide
	1,1,1-Trifluoro-N-(2-methyl-4-(phenylsulfonyl)phenyl)methanesulfonamide
	1,1,1-Trifluoro-N-[2-methyl-4-(phenylsulphonyl)phenyl]methanesulfonamide
	1,1,1-trifluoro-N-(4-phenylsulphonyl-o-tolyl)methanesulphonamide
	2-Methyl-4-(phenylsulfonyl)trifluoromethanesulfonanilide
	Destun
	MBR 8251
	Methanesulfonamide, 1,1,1-trifluoro-N-[2-methyl-4-(phenylsulfonyl)phenyl]-
	Methanesulfonamide, N-(4-phenylsulfonyl-o-tolyl)-1,1,1-trifluoro-
	SB 1528
Inchi:	InChI=1S/C14H12F3NO4S2/c1-10-9-12(23(19,20)11-5-3-2-4-6-11)7-8-13(10)18-24(21,22
InchiKey:	WHTBVLXUSXVMEV-UHFFFAOYSA-N
Formula:	C14H12F3NO4S2
SMILES:	Cc1cc(S(=O)(=O)c2ccccc2)ccc1NS(=O)(=O)C(F)(F)F
Mol. weight [g/mol]:	379.38
CAS:	37924-13-3

Physical Properties

Property code	Value	Unit	Source
gf	-1156.72	kJ/mol	Joback Method
hf	-1332.48	kJ/mol	Joback Method
hfus	49.00	kJ/mol	Joback Method
hvap	92.59	kJ/mol	Joback Method
log10ws	-3.80		Estimated Solubility Method
logp	3.089		Crippen Method
mcvol	232.070	ml/mol	McGowan Method
pc	3368.44	kPa	Joback Method
tb	723.35	K	Joback Method
tc	928.87	K	Joback Method
tf	419.13 ± 0.20	K	NIST Webbook
vc	0.933	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	676.89	J/mol×K	894.62	Joback Method
cpg	622.96	J/mol×K	723.35	Joback Method
cpg	636.08	J/mol×K	757.60	Joback Method
cpg	648.00	J/mol×K	791.86	Joback Method
cpg	658.75	J/mol×K	826.11	Joback Method
cpg	668.37	J/mol×K	860.36	Joback Method
cpg	684.33	J/mol×K	928.87	Joback Method
hfust	31.79	kJ/mol	418.40	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method: https://en.wikipedia.org/wiki/Joback_method
Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C37924133&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
hfust: Enthalpy of fusion at a given temperature
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