Tolylfluanid

Other names:	Methanesulfenamide, 1,1-dichloro-N-[(dimethylamino)sulfonyl]-1-fluoro-N-(4-methylphenyl)-
	Sulfamide, N-((dichlorofluoromethyl)thio)-N',N'-dimethyl-N-(p-tolyl)-
	BAY 49854
	BAY 5212
	BAY 5712a
	Bayer 49854
	Bayer 5712a
	Dichlofluanid-methyl
	N'-Dichlorofluoromethylthio-N,N-dimethyl-N'-(4-tolyl)sulfamide
	N,N-Dimethyl-N-(4-tolyl)-N-(dichlorofluor-methylthio)-sulfamide
	N,N-Dimethyl-N'-(4-tolyl)-N'-(dichlorfluormethylthio)-sulfamid
	Euparen M
	Tolylfluanide
	KUE 13183b
	Methanesulfanenamide, 1,1-dichloro-N-((dimethylamino)sulfonyl)-1-fluoro-N-(4-methylphenyl)-
	1,1-Dichloro-N-((dimethylamino)sulfonyl)-1-fluoro-N-(4-methylphenyl)methanesulfonamid
	Tolyfluanid
	Tolyfluanide
	dichloro-N-[(dimethylamino)sulphonyl]fluoro-N-(p-tolyl)methanesulphenamide
Inchi:	InChI=1S/C10H13Cl2FN2O2S2/c1-8-4-6-9(7-5-8)15(18-10(11,12)13)19(16,17)14(2)3/h4-
InchiKey:	HYVWIQDYBVKITD-UHFFFAOYSA-N
Formula:	C10H13Cl2FN2O2S2
SMILES:	Cc1ccc(N(SC(F)(Cl)Cl)S(=O)(=O)N(C)C)cc1
Mol. weight [g/mol]:	347.26
CAS:	731-27-1

Physical Properties

Property code	Value	Unit	Source
gf	-293.59	kJ/mol	Joback Method
hf	-537.43	kJ/mol	Joback Method
hfus	40.92	kJ/mol	Joback Method
hvap	76.99	kJ/mol	Joback Method
log10ws	-4.29		Crippen Method
logp	3.314		Crippen Method
mcvol	218.650	ml/mol	McGowan Method
pc	3107.10	kPa	Joback Method
rinpol	2016.00		NIST Webbook

rinpol	2073.00		NIST Webbook
tb	672.20	K	Joback Method
tc	893.42	K	Joback Method
tf	442.15	K	Joback Method
vc	0.808	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	529.01	J/mol×K	672.20	Joback Method
cpg	542.32	J/mol×K	709.07	Joback Method
cpg	554.46	J/mol×K	745.94	Joback Method
cpg	565.47	J/mol×K	782.81	Joback Method
cpg	575.42	J/mol×K	819.68	Joback Method
cpg	584.37	J/mol×K	856.55	Joback Method
cpg	592.36	J/mol×K	893.42	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=C731271&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume