Fluoridamid

Other names:	Acetamide, N-[4-methyl-3-[[(trifluoromethyl)sulfonyl]amino]phenyl]-
	Sustar
	Toluene-2,4-diamine, N4-acetyl-N2-trifluoromethylsulfonyl-
	MBR 6033
	(N-4-Methyl-(((1,1,1-trifluoromethyl)sulfonyl)amino)phenyl)acetamide
	Sustar 2S
	3-Trifluoromethylsulfonamido-p-acetotoluidide
	N-(4-Methyl-3-([(trifluoromethyl)sulfonyl]amino)phenyl)acetamide
Inchi:	InChI=1S/C10H11F3N2O3S/c1-6-3-4-8(14-7(2)16)5-9(6)15-19(17,18)10(11,12)13/h3-5,1
InchiKey:	CUYDUAXYJJPSRK-UHFFFAOYSA-N
Formula:	C10H11F3N2O3S
SMILES:	CC(=O)Nc1ccc(C)c(NS(=O)(=O)C(F)(F)F)c1
Mol. weight [g/mol]:	296.27
CAS:	47000-92-0

Physical Properties

Property code	Value	Unit	Source
gf	-873.80	kJ/mol	Joback Method
hf	-1092.21	kJ/mol	Joback Method
hfus	39.92	kJ/mol	Joback Method
hvap	75.96	kJ/mol	Joback Method
log10ws	-3.14		Crippen Method
logp	2.215		Crippen Method
mcvol	182.930	ml/mol	McGowan Method
pc	3269.04	kPa	Joback Method
tb	661.41	K	Joback Method
tc	855.64	K	Joback Method
tf	456.31 ± 0.20	K	NIST Webbook
vc	0.733	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	481.69	J/mol×K	661.41	Joback Method

cpg	493.32	J/mol×K	693.78	Joback Method
cpg	504.11	J/mol×K	726.15	Joback Method
cpg	514.09	J/mol×K	758.53	Joback Method
cpg	523.28	J/mol×K	790.90	Joback Method
cpg	531.71	J/mol×K	823.27	Joback Method
cpg	539.40	J/mol×K	855.64	Joback Method
hfust	40.47	kJ/mol	455.70	NIST Webbook

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=C47000920&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
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