Acetamide, N-[2,4-dimethyl-5-[[(trifluoromethyl)sulfonyl]amino

Other names: 2',4'-dimethyl-5'-(trifluoromethanesulphonamido)acetanilide
5'-(Trifluoromethanesulphonamide)acet-2',4-xylidide
5-Acetamido-2,4-dimethyltrifluoromethanesulfonanilide
Acetanilide, 2',4'-dimethyl-5-((trifluoromethyl)sulfonamido)-
Embark
Embark 2S
Embark plant growth regulator
MBR 12325
Mefluidide
Mowchem
N-(2,4-Dimethyl-5-(((trifluoromethyl)sulfonyl)amino)phenyl)acetamide
N-[2,4-dimethyl-5-(trifluoromethylsulfonylamino)phenyl]acetamide
Trimcut
VEL 3973
Vistar
Vistar herbicide

Inchi: InChI=1S/C11H13F3N2O3S/c1-6-4-7(2)10(5-9(6)15-8(3)17)16-20(18,19)11(12,13)14/h4-

InchiKey: OKIBNKKYNPBDRS-UHFFFAOYSA-N

Formula: C11H13F3N2O3S

SMILES: CC(=O)Nc1cc(NS(=O)(=O)C(F)(F)F)c(C)cc1C

Mol. weight [g/mol]: 310.29

CAS: 53780-34-0

Physical Properties

Property code	Value	Unit	Source
gf	-875.01	kJ/mol	Joback Method
hf	-1124.32	kJ/mol	Joback Method
hfus	42.12	kJ/mol	Joback Method
hvap	78.85	kJ/mol	Joback Method
log10ws	-3.24		Estimated Solubility Method
log10ws	-3.24		Aqueous Solubility Prediction Method
logp	2.523		Crippen Method
mcvol	197.020	ml/mol	McGowan Method
pc	2890.51	kPa	Joback Method
tb	689.27	K	Joback Method

tc	882.49	K	Joback Method
tf	457.48 ± 0.20	K	NIST Webbook
vc	0.788	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	531.37	J/mol×K	689.27	Joback Method
cpg	543.31	J/mol×K	721.47	Joback Method
cpg	554.42	J/mol×K	753.68	Joback Method
cpg	564.71	J/mol×K	785.88	Joback Method
cpg	574.20	J/mol×K	818.09	Joback Method
cpg	582.91	J/mol×K	850.29	Joback Method
cpg	590.88	J/mol×K	882.49	Joback Method
hfust	37.66	kJ/mol	457.30	NIST Webbook

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
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=C53780340&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