4-Methylthioamphetamine-M/artifact (sulfoxide) acetylated

Inchi: InChI=1S/C12H17NO3S/c1-9(13-10(2)14)8-11-4-6-12(7-5-11)17(3,15)16/h4-7,9H,8H2,1-

InchiKey: VMGFUUVUFWMVAZ-UHFFFAOYSA-N

Formula: C12H17NO3S

SMILES: CC(=O)NC(C)Cc1ccc(S(C)(=O)=O)cc1

Mol. weight [g/mol]: 255.33

Physical Properties

Property code	Value	Unit	Source
gf	-357.57	kJ/mol	Joback Method
hf	-583.69	kJ/mol	Joback Method
hfus	35.04	kJ/mol	Joback Method
hvap	76.67	kJ/mol	Joback Method
log10ws	-2.30		Crippen Method
logp	1.157		Crippen Method
mcvol	195.820	ml/mol	McGowan Method
pc	3035.62	kPa	Joback Method
rinpol	2360.00		NIST Webbook
rinpol	2360.00		NIST Webbook
tb	657.00	K	Joback Method
tc	862.95	K	Joback Method
tf	390.09	K	Joback Method
vc	0.760	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	506.11	J/mol×K	657.00	Joback Method
cpg	520.96	J/mol×K	691.32	Joback Method
cpg	534.83	J/mol×K	725.65	Joback Method
cpg	547.74	J/mol×K	759.97	Joback Method
cpg	559.70	J/mol×K	794.30	Joback Method
cpg	570.73	J/mol×K	828.62	Joback Method
cpg	580.86	J/mol×K	862.95	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R413219&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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