N-(1-methyl-2-[4-(methylsulfanyl)phenyl]ethyl)ace

Other names: 4-methylthioamphetamine acetylated
Inchi: InChI=1S/C12H17NOS/c1-9(13-10(2)14)8-11-4-6-12(15-3)7-5-11/h4-7,9H,8H2,1-3H3,(H,
InchiKey: BKTUHYUDOIRFKH-UHFFFAOYSA-N
Formula: C12H17NOS
SMILES: CSc1ccc(CC(C)N=C(C)O)cc1
Mol. weight [g/mol]: 223.33
CAS: 634607-26-4

Physical Properties

Property code	Value	Unit	Source
hf	-109.16	kJ/mol	Joback Method
hvap	71.75	kJ/mol	Joback Method
log10ws	-3.37		Crippen Method
logp	3.316		Crippen Method
mcvol	184.080	ml/mol	McGowan Method
pc	2410.00	kPa	Joback Method
rinpol	1700.00		NIST Webbook
rinpol	1700.00		NIST Webbook
tb	742.70	K	Joback Method
tc	966.71	K	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C634607264&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

Legend

hf:	Enthalpy of formation 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