

1-(4-Methylthiophenyl)-2-propanol, acetate

Other names:	4-Methylthioamphetamine -M (deamino-HO-) acetylated
Inchi:	InChI=1S/C12H16O2S/c1-9(14-10(2)13)8-11-4-6-12(15-3)7-5-11/h4-7,9H,8H2,1-3H3
InchiKey:	DAYOFLPZRYAPSP-UHFFFAOYSA-N
Formula:	C12H16O2S
SMILES:	CSc1ccc(CC(C)OC(C)=O)cc1
Mol. weight [g/mol]:	224.32

Physical Properties

Property code	Value	Unit	Source
gf	-50.30	kJ/mol	Joback Method
hf	-274.16	kJ/mol	Joback Method
hfus	23.88	kJ/mol	Joback Method
hvap	60.83	kJ/mol	Joback Method
log10ws	-3.25		Crippen Method
logp	2.903		Crippen Method
mvol	179.970	ml/mol	McGowan Method
pc	2543.05	kPa	Joback Method
rinpol	1460.00		NIST Webbook
rinpol	1460.00		NIST Webbook
tb	650.25	K	Joback Method
tc	878.49	K	Joback Method
tf	355.50	K	Joback Method
vc	0.671	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	448.59	J/molxK	650.25	Joback Method
cpg	463.72	J/molxK	688.29	Joback Method
cpg	477.86	J/molxK	726.33	Joback Method
cpg	491.02	J/molxK	764.37	Joback Method
cpg	503.21	J/molxK	802.41	Joback Method
cpg	514.45	J/molxK	840.45	Joback Method
cpg	524.75	J/molxK	878.49	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360380&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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