1-(4-methylthiophenyl)-2-propanone

Other names: 4-Methylthioamphetamine -M (deamino oxo-)
Inchi: InChI=1S/C10H12OS/c1-8(11)7-9-3-5-10(12-2)6-4-9/h3-6H,7H2,1-2H3
InchiKey: RYFZDEIJXAESAA-UHFFFAOYSA-N
Formula: C10H12OS
SMILES: CSc1ccc(CC(C)=O)cc1
Mol. weight [g/mol]: 180.27

Physical Properties

Property code	Value	Unit	Source
gf	40.30	kJ/mol	Joback Method
hf	-95.38	kJ/mol	Joback Method
hfus	21.04	kJ/mol	Joback Method
hvap	54.36	kJ/mol	Joback Method
log10ws	-2.72		Crippen Method
logp	2.540		Crippen Method
mcvol	145.920	ml/mol	McGowan Method
pc	3149.09	kPa	Joback Method
tb	582.51	K	Joback Method
tc	818.40	K	Joback Method
tf	325.73	K	Joback Method
vc	0.547	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	326.39	J/mol×K	582.51	Joback Method
cpg	340.06	J/mol×K	621.83	Joback Method
cpg	352.82	J/mol×K	661.14	Joback Method
cpg	364.70	J/mol×K	700.46	Joback Method
cpg	375.74	J/mol×K	739.77	Joback Method
cpg	385.95	J/mol×K	779.09	Joback Method
cpg	395.37	J/mol×K	818.40	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U378998&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume