Amphetamine, 3'-fluoro-4'-methoxy

Inchi: InChI=1S/C10H14FNO/c1-7(12)5-8-3-4-10(13-2)9(11)6-8/h3-4,6-7H,5,12H2,1-2H3
InchiKey: WYEYFMJGWCHRCH-UHFFFAOYSA-N
Formula: C10H14FNO
SMILES: COc1ccc(CC(C)N)cc1F
Mol. weight [g/mol]: 183.22

Physical Properties

Property code	Value	Unit	Source
gf	-109.33	kJ/mol	Joback Method
hf	-335.96	kJ/mol	Joback Method
hfus	20.86	kJ/mol	Joback Method
hvap	53.30	kJ/mol	Joback Method
log10ws	-2.69		Crippen Method
logp	1.724		Crippen Method
mcvol	145.620	ml/mol	McGowan Method
pc	2847.48	kPa	Joback Method
rinpol	1363.00		NIST Webbook
rinpol	1363.00		NIST Webbook
tb	558.62	K	Joback Method
tc	768.15	K	Joback Method
tf	345.00	K	Joback Method
vc	0.546	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	348.90	J/mol×K	558.62	Joback Method
cpg	362.57	J/mol×K	593.54	Joback Method
cpg	375.53	J/mol×K	628.46	Joback Method
cpg	387.80	J/mol×K	663.39	Joback Method
cpg	399.38	J/mol×K	698.31	Joback Method
cpg	410.30	J/mol×K	733.23	Joback Method
cpg	420.55	J/mol×K	768.15	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R586144&Units=SI

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