

4-fluoromethamphetamine

Other names:	4-FMA p-Fluoromethamphetamine
Inchi:	InChI=1S/C10H14FN/c1-8(12-2)7-9-3-5-10(11)6-4-9/h3-6,8,12H,7H2,1-2H3
InchiKey:	YCWZPIHKUYZTFM-UHFFFAOYSA-N
Formula:	C10H14FN
SMILES:	CNC(C)Cc1ccc(F)cc1
Mol. weight [g/mol]:	167.22
CAS:	351-03-1

Physical Properties

Property code	Value	Unit	Source
gf	28.24	kJ/mol	Joback Method
hf	-172.59	kJ/mol	Joback Method
hfus	19.96	kJ/mol	Joback Method
hvap	46.02	kJ/mol	Joback Method
log10ws	-2.74		Crippen Method
logp	1.976		Crippen Method
mcvol	139.750	ml/mol	McGowan Method
pc	2811.36	kPa	Joback Method
rinpol	1278.30		NIST Webbook
tb	508.86	K	Joback Method
tc	710.38	K	Joback Method
tf	279.65	K	Joback Method
vc	0.534	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	313.38	J/mol×K	508.86	Joback Method
cpg	327.86	J/mol×K	542.45	Joback Method
cpg	341.56	J/mol×K	576.03	Joback Method
cpg	354.49	J/mol×K	609.62	Joback Method
cpg	366.68	J/mol×K	643.21	Joback Method
cpg	378.17	J/mol×K	676.80	Joback Method

Sources

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=C351031&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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