

3-fluoroamphetamine

Other names:	Amphetamine, 3'-fluoro
Inchi:	InChI=1S/C9H12FN/c1-7(11)5-8-3-2-4-9(10)6-8/h2-4,6-7H,5,11H2,1H3
InchiKey:	PIOCLGPCMNPZFT-UHFFFAOYSA-N
Formula:	C9H12FN
SMILES:	CC(N)Cc1cccc(F)c1
Mol. weight [g/mol]:	153.20

Physical Properties

Property code	Value	Unit	Source
hf	-204.22	kJ/mol	Cheméo Relay (1.0)
hfus	17.47	kJ/mol	Joback Method
hvap	57.47	kJ/mol	Cheméo Relay (1.0)
ie	8.80	eV	Cheméo Relay (1.0)
log10ws	-1.28		Cheméo Relay (1.0)
logp	1.715		Crippen Method
mcvol	125.660	ml/mol	McGowan Method
rinpol	1112.00		NIST Webbook
rinpol	1112.00		NIST Webbook
tb	465.84	K	Cheméo Relay (1.0)
tf	277.95	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	280.09	J/mol×K	508.34	Joback Method
cpg	293.46	J/mol×K	544.01	Joback Method
cpg	306.04	J/mol×K	579.68	Joback Method
cpg	317.87	J/mol×K	615.36	Joback Method
cpg	328.97	J/mol×K	651.03	Joback Method
cpg	339.38	J/mol×K	686.70	Joback Method
cpg	349.12	J/mol×K	722.37	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1716592&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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