Phenethylamine, o-fluoro-«alpha»-methyl-

Other names: o-Fluoro-«alpha»-methylphenethylamine
2-Fluoroamphetamine
Inchi: InChI=1S/C9H12FN/c1-7(11)6-8-4-2-3-5-9(8)10/h2-5,7H,6,11H2,1H3
InchiKey: GDSXNLDTQFFIEU-UHFFFAOYSA-N
Formula: C9H12FN
SMILES: CC(N)Cc1ccccc1F
Mol. weight [g/mol]: 153.20
CAS: 1716-60-5

Physical Properties

Property code	Value	Unit	Source
gf	-3.12	kJ/mol	Joback Method
hf	-171.63	kJ/mol	Joback Method
hfus	17.47	kJ/mol	Joback Method
hvap	48.00	kJ/mol	Joback Method
log10ws	-2.57		Crippen Method
logp	1.715		Crippen Method
mcvol	125.660	ml/mol	McGowan Method
pc	3280.28	kPa	Joback Method
rinpol	1228.00		NIST Webbook
rinpol	1228.00		NIST Webbook
tb	508.34	K	Joback Method
tc	722.37	K	Joback Method
tf	298.98	K	Joback Method
vc	0.472	m3/kmol	Joback Method

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=C1716605&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume