

n-Heptafluorobutyryl-methamphetamine

Other names:	Methamphetamine, HFB Methamphetamine, HFBA
Inchi:	InChI=1S/C14H14F7NO/c1-9(8-10-6-4-3-5-7-10)22(2)11(23)12(15,16)13(17,18)14(19,20)
InchiKey:	WRGPIHJTEFMXOA-UHFFFAOYSA-N
Formula:	C14H14F7NO
SMILES:	CC(Cc1ccccc1)N(C)C(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	345.26
CAS:	156572-16-6

Physical Properties

Property code	Value	Unit	Source
gf	-1196.32	kJ/mol	Joback Method
hf	-1545.11	kJ/mol	Joback Method
hfus	26.47	kJ/mol	Joback Method
hvap	47.83	kJ/mol	Joback Method
log10ws	-4.53		Crippen Method
logp	3.909		Crippen Method
mcvol	208.300	ml/mol	McGowan Method
pc	1707.53	kPa	Joback Method
tb	597.47	K	Joback Method
tc	773.64	K	Joback Method
tf	352.75	K	Joback Method
vc	0.823	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	570.66	J/mol×K	597.47	Joback Method
cpg	585.52	J/mol×K	626.83	Joback Method
cpg	599.31	J/mol×K	656.19	Joback Method
cpg	612.09	J/mol×K	685.55	Joback Method
cpg	623.93	J/mol×K	714.92	Joback Method
cpg	634.91	J/mol×K	744.28	Joback Method
cpg	645.09	J/mol×K	773.64	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C156572166&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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

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