Methylenedioxymethamphetamine, n-heptafluorobutyryl deriv.

Other names: MDMA, HFB
Inchi: InChI=1S/C15H14F7NO3/c1-8(5-9-3-4-10-11(6-9)26-7-25-10)23(2)12(24)13(16,17)14(18
InchiKey: ZGHICVNRTPSTFX-UHFFFAOYSA-N
Formula: C15H14F7NO3
SMILES: CC(Cc1ccc2c(c1)OCO2)N(C)C(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 389.27
CAS: 156572-21-3

Physical Properties

Property code	Value	Unit	Source
gf	-1310.94	kJ/mol	Joback Method
hf	-1759.55	kJ/mol	Joback Method
hfus	41.31	kJ/mol	Joback Method
hvap	60.62	kJ/mol	Joback Method
log10ws	-4.74		Crippen Method
logp	3.638		Crippen Method
mcvol	223.270	ml/mol	McGowan Method
pc	1734.67	kPa	Joback Method
tb	695.62	K	Joback Method
tc	882.57	K	Joback Method
tf	464.38	K	Joback Method
vc	0.878	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	667.89	J/mol×K	695.62	Joback Method
cpg	680.66	J/mol×K	726.78	Joback Method
cpg	692.47	J/mol×K	757.94	Joback Method
cpg	703.41	J/mol×K	789.09	Joback Method
cpg	713.59	J/mol×K	820.25	Joback Method
cpg	723.09	J/mol×K	851.41	Joback Method
cpg	732.02	J/mol×K	882.57	Joback Method

Sources

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=C156572213&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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