Ephedrine,N,O-bis(heptafluorobutyryl) deriv.

Other names:	Ephedrine, N,O-bis-HFB
	N,O-Bis(heptafluorobutyryl)ephedrine
	Ephedrine, HFB
	Ephedrine, HFBA
Inchi:	InChI=1S/C18H13F14NO3/c1-8(33(2)11(34)13(19,20)15(23,24)17(27,28)29)10(9-6-4-3-5
InchiKey:	BCMWTPKOZMDVHA-UHFFFAOYSA-N
Formula:	C18H13F14NO3
SMILES:	CC(C(OC(=O)C(F)(F)C(F)(F)C(F)(F)F)c1ccccc1)N(C)C(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	557.28
CAS:	66091-19-8

Physical Properties

Property code	Value	Unit	Source
gf	-2754.15	kJ/mol	Joback Method
hf	-3276.77	kJ/mol	Joback Method
hfus	35.41	kJ/mol	Joback Method
hvap	55.89	kJ/mol	Joback Method
log10ws	-6.82		Crippen Method
logp	5.784		Crippen Method
mcvol	284.490	ml/mol	McGowan Method
pc	1105.21	kPa	Joback Method
tb	750.04	K	Joback Method
tc	922.45	K	Joback Method
tf	466.38	K	Joback Method
vc	1.157	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	894.50	J/mol×K	750.04	Joback Method
cpg	906.32	J/mol×K	778.77	Joback Method
cpg	917.19	J/mol×K	807.51	Joback Method
cpg	927.21	J/mol×K	836.24	Joback Method
cpg	936.47	J/mol×K	864.98	Joback Method

cpg	945.08	J/mol×K	893.71	Joback Method
cpg	953.13	J/mol×K	922.45	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=C66091198&Units=SI&Mask=3FFF
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume