DL-Metanephrine, N,O,O'-tris(trifluoroacetyl)-

Other names: Metanephrine, TFA
Inchi: InChI=1S/C16H12F9NO6/c1-26(11(27)14(17,18)19)6-10(32-13(29)16(23,24)25)7-3-4-8(9
InchiKey: AIKLVQAXEMSHQZ-UHFFFAOYSA-N
Formula: C16H12F9NO6
SMILES: COc1cc(C(CN(C)C(=O)C(F)(F)F)OC(=O)C(F)(F)F)ccc1OC(=O)C(F)(F)F
Mol. weight [g/mol]: 485.26

Physical Properties

Property code	Value	Unit	Source
gf	-2161.20	kJ/mol	Joback Method
hf	-2623.37	kJ/mol	Joback Method
hfus	43.80	kJ/mol	Joback Method
hvap	72.69	kJ/mol	Joback Method
log10ws	-4.46		Crippen Method
logp	3.330		Crippen Method
mcvol	260.770	ml/mol	McGowan Method
pc	1416.50	kPa	Joback Method
rinpol	1652.00		NIST Webbook
rinpol	1652.00		NIST Webbook
rinpol	1615.00		NIST Webbook
tb	826.73	K	Joback Method
tc	1015.28	K	Joback Method
tf	568.06	K	Joback Method
vc	1.036	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	803.60	J/mol×K	826.73	Joback Method
cpg	813.76	J/mol×K	858.16	Joback Method
cpg	823.04	J/mol×K	889.58	Joback Method
cpg	831.48	J/mol×K	921.01	Joback Method
cpg	839.14	J/mol×K	952.43	Joback Method
cpg	846.06	J/mol×K	983.86	Joback Method

cpg	852.29	J/mol×K	1015.28	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375726&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

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