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

Inchi: InChI=1S/C19H12F15NO6/c1-35(11(36)14(20,21)17(26,27)28)6-10(41-13(38)16(24,25)1

InchiKey: GDOLGVPSPFQELD-UHFFFAOYSA-N

Formula: C19H12F15NO6

SMILES: COc1cc(C(CN(C)C(=O)C(F)(F)C(F)(F)F)OC(=O)C(F)(F)C(F)(F)F)ccc1OC(=O)C(F)(F)C(F

Mol. weight [g/mol]: 635.28

Physical Properties

Property code	Value	Unit	Source
gf	-3296.28	kJ/mol	Joback Method
hf	-3888.20	kJ/mol	Joback Method
hfus	47.80	kJ/mol	Joback Method
hvap	70.58	kJ/mol	Joback Method
log10ws	-6.65		Crippen Method
logp	5.236		Crippen Method
mcvol	313.660	ml/mol	McGowan Method
pc	1002.71	kPa	Joback Method
rinpol	1648.00		NIST Webbook
rinpol	1648.00		NIST Webbook
tb	881.30	K	Joback Method
tc	1080.72	K	Joback Method
tf	612.67	K	Joback Method
vc	1.280	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1018.84	J/mol×K	881.30	Joback Method
cpg	1028.88	J/mol×K	914.54	Joback Method
cpg	1038.03	J/mol×K	947.77	Joback Method
cpg	1046.43	J/mol×K	981.01	Joback Method
cpg	1054.20	J/mol×K	1014.25	Joback Method
cpg	1061.45	J/mol×K	1047.48	Joback Method
cpg	1068.31	J/mol×K	1080.72	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=U375725&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume