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

Inchi: InChI=1S/C22H12F21NO6/c1-44(11(45)14(23,24)17(29,30)20(35,36)37)6-10(50-13(47)1

InchiKey: DQVQZQMDDNPFGN-UHFFFAOYSA-N

Formula: C22H12F21NO6

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

Mol. weight [g/mol]: 785.30

Physical Properties

Property code	Value	Unit	Source
gf	-4431.36	kJ/mol	Joback Method
hf	-5153.03	kJ/mol	Joback Method
hfus	51.81	kJ/mol	Joback Method
hvap	68.47	kJ/mol	Joback Method
log10ws	-8.85		Crippen Method
logp	7.142		Crippen Method
mcvol	366.550	ml/mol	McGowan Method
pc	746.92	kPa	Joback Method
rinpol	1715.00		NIST Webbook
tb	935.87	K	Joback Method
tc	1167.46	K	Joback Method
tf	657.28	K	Joback Method
vc	1.522	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1234.50	J/mol×K	935.87	Joback Method
cpg	1245.61	J/mol×K	974.47	Joback Method
cpg	1255.99	J/mol×K	1013.07	Joback Method
cpg	1265.95	J/mol×K	1051.67	Joback Method
cpg	1275.75	J/mol×K	1090.26	Joback Method
cpg	1285.70	J/mol×K	1128.86	Joback Method
cpg	1296.09	J/mol×K	1167.46	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375724&Units=SI

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