

(.+/-.)-Epinephrine, N,O,O',O''-tetrakis(heptafluorobutyryl)-

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C25H9F28NO7/c1-54(10(55)14(26,27)18(34,35)22(42,43)44)5-9(61-13(58)17(

ZHEKJTDOISUKEC-UHFFFAOYSA-N

C25H9F28NO7

CN(CC(OC(=O)C(F)(F)C(F)(F)C(F)(F)F)c1ccc(OC(=O)C(F)(F)C(F)(F)C(F)(F)F)c(OC(=O)

967.30

Physical Properties

Property code	Value	Unit	Source
gf	-5890.17	kJ/mol	Joback Method
hf	-6726.55	kJ/mol	Joback Method
hfus	60.50	kJ/mol	Joback Method
hvap	72.28	kJ/mol	Joback Method
log10ws	-11.17		Crippen Method
logp	8.872		Crippen Method
mcvol	422.780	ml/mol	McGowan Method
pc	582.88	kPa	Joback Method
rinpol	1618.00		NIST Webbook
rinpol	1618.00		NIST Webbook
tb	1043.58	K	Joback Method
tc	1378.88	K	Joback Method
tf	752.41	K	Joback Method
vc	1.790	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1462.26	J/mol×K	1043.58	Joback Method
cpg	1477.98	J/mol×K	1099.46	Joback Method
cpg	1495.10	J/mol×K	1155.35	Joback Method
cpg	1514.81	J/mol×K	1211.23	Joback Method
cpg	1538.26	J/mol×K	1267.12	Joback Method
cpg	1566.62	J/mol×K	1323.00	Joback Method
cpg	1601.08	J/mol×K	1378.88	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375690&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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