

(-)-Norepinephrine, N,O,O',O''-tetrakis(trifluoroacetyl)-

Inchi: InChI=1S/C16H7F12NO7/c17-13(18,19)9(30)29-4-8(36-12(33)16(26,27)28)5-1-2-6(34-10)3
InchiKey: BPWJTVGJINOJLL-UHFFFAOYSA-N
Formula: C16H7F12NO7
SMILES: O=C(NCC(OC(=O)C(F)(F)F)c1ccc(OC(=O)C(F)(F)F)c(OC(=O)C(F)(F)F)c1)C(F)(F)F
Mol. weight [g/mol]: 553.21

Physical Properties

Property code	Value	Unit	Source
gf	-2893.10	kJ/mol	Joback Method
hf	-3347.09	kJ/mol	Joback Method
hfus	49.30	kJ/mol	Joback Method
hvap	80.08	kJ/mol	Joback Method
log10ws	-5.51		Crippen Method
logp	3.447		Crippen Method
mcvol	267.650	ml/mol	McGowan Method
pc	1376.84	kPa	Joback Method
rinpol	1523.00		NIST Webbook
tb	912.91	K	Joback Method
tc	1117.86	K	Joback Method
tf	642.37	K	Joback Method
vc	1.103	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	842.92	J/mol×K	912.91	Joback Method
cpg	850.23	J/mol×K	947.07	Joback Method
cpg	856.69	J/mol×K	981.23	Joback Method
cpg	862.37	J/mol×K	1015.39	Joback Method
cpg	867.35	J/mol×K	1049.54	Joback Method
cpg	871.71	J/mol×K	1083.70	Joback Method
cpg	875.53	J/mol×K	1117.86	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=U375717&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

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