Butanoic acid, heptafluoro-, 4-[2-[(2,2,3,3,4,4,4-heptafluoro-1-oxobutyl)amino]e ester

Othernames: Dopamine, tris (N,O,O-HFB)
3-Hydroxytyramine, N,O,O'-tris(heptafluorobutyryl)-
Inchi: InChI=1S/C20H8F21NO5/c21-12(22,15(27,28)18(33,34)35)9(43)42-4-3-6-1-2-7(46-10(44
InchiKey: HQCGNAGTHKEFMI-UHFFFAOYSA-N
Formula: C20H8F21NO5
SMILES: O=C(NCCc1ccc(OC(=O)C(F)(F)C(F)(F)C(F)(F)F)c(OC(=O)C(F)(F)C(F)(F)C(F)(F)F)c1)C(
Mol. weight [g/mol]: 741.25
CAS: 55538-89-1

Physical Properties

Property code	Value	Unit	Source
gf	-4362.15	kJ/mol	Joback Method
hf	-4988.31	kJ/mol	Joback Method
hfus	51.04	kJ/mol	Joback Method
hvap	66.39	kJ/mol	Joback Method
log10ws	-9.09		Crippen Method
logp	6.655		Crippen Method
mcvol	332.500	ml/mol	McGowan Method
pc	843.58	kPa	Joback Method
rinpol	1660.00		NIST Webbook
tb	905.86	K	Joback Method
tc	1120.97	K	Joback Method
tf	647.70	K	Joback Method
vc	1.415	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1105.97	J/mol×K	905.86	Joback Method
cpg	1115.28	J/mol×K	941.71	Joback Method
cpg	1123.97	J/mol×K	977.56	Joback Method
cpg	1132.25	J/mol×K	1013.42	Joback Method
cpg	1140.36	J/mol×K	1049.27	Joback Method
cpg	1148.54	J/mol×K	1085.12	Joback Method

cpg	1157.01	J/mol×K	1120.97	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=C55538891&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