

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

Other names: Octopamine, tris-(N,O,O-HFB)-
(.+/-)-Octopamine, N,O,O'-tris(heptafluorobutyl)-

Inchi: 4-[(2,2,3,3,4,4,4-Heptafluorobutanoyl)amino]-1-[(2,2,3,3,4,4,4-heptafluorobutanoyl)oxy]butane
InchiKey: HIUHYYIAZBIILC-UHFFFAOYSA-N
Formula: C₂₀H₈F₂₁NO₅
SMILES: O=C(NCC(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)cc1)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 741.25
CAS: 55538-87-9

Physical Properties

Property code	Value	Unit	Source
gf	-4354.96	kJ/mol	Joback Method
hf	-4982.12	kJ/mol	Joback Method
hfus	47.91	kJ/mol	Joback Method
hvap	65.34	kJ/mol	Joback Method
log10ws	-8.93		Crippen Method
logp	6.791		Crippen Method
mcvol	332.500	ml/mol	McGowan Method
pc	854.96	kPa	Joback Method
rinpol	1570.00		NIST Webbook
rinpol	1570.00		NIST Webbook
tb	900.44	K	Joback Method
tc	1112.16	K	Joback Method
tf	620.18	K	Joback Method
vc	1.409	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1108.26	J/molxK	900.44	Joback Method
cpg	1117.48	J/molxK	935.73	Joback Method
cpg	1126.05	J/molxK	971.01	Joback Method
cpg	1134.19	J/molxK	1006.30	Joback Method

cpg	1142.13	J/mol×K	1041.59	Joback Method
cpg	1150.10	J/mol×K	1076.87	Joback Method
cpg	1158.33	J/mol×K	1112.16	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C55538879&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

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