

4-[2-Bis(trifluoroacetyl)amino-1-(trifluoroacetyloxy)phenyl]-2-bis(trifluoroacetyl)aminoethanol trifluoroacetate

Other names: 1-(4-(Trifluoroacetyloxyphenyl)-2-bis(trifluoroacetyl)aminoethanol trifluoroacetate
Inchi: InChI=1S/C16H7F12NO6/c17-13(18,19)9(30)29(10(31)14(20,21)22)5-8(35-12(33)16(26,27)34)32
InchiKey: FLDZGSDPEIXVCA-UHFFFAOYSA-N
Formula: C16H7F12NO6
SMILES: O=C(Oc1ccc(C(CN(C(=O)C(F)(F)F)C(=O)C(F)(F)F)OC(=O)C(F)(F)F)cc1)C(F)(F)F
Mol. weight [g/mol]: 537.21

Physical Properties

Property code	Value	Unit	Source
gf	-2757.08	kJ/mol	Joback Method
hf	-3189.34	kJ/mol	Joback Method
hfus	46.42	kJ/mol	Joback Method
hvap	72.62	kJ/mol	Joback Method
log10ws	-5.19		Crippen Method
logp	3.781		Crippen Method
mcvol	261.780	ml/mol	McGowan Method
pc	1394.37	kPa	Joback Method
rinpol	1343.00		NIST Webbook
tb	847.78	K	Joback Method
tc	1038.61	K	Joback Method
tf	587.43	K	Joback Method
vc	1.067	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	812.52	J/molxK	847.78	Joback Method
cpg	820.78	J/molxK	879.59	Joback Method
cpg	828.25	J/molxK	911.39	Joback Method
cpg	835.01	J/molxK	943.20	Joback Method
cpg	841.14	J/molxK	975.00	Joback Method
cpg	846.74	J/molxK	1006.81	Joback Method
cpg	851.87	J/molxK	1038.61	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373480&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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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