

2-Hydroxy-2-phenylethylamine di(trifluoroacetyl)-

Other names:	2-Amino-1-phenylethanol, N,O-bis(trifluoroacetyl)- 1-Phenyl-2-[(trifluoroacetyl)amino]ethyl trifluoroacetate
Inchi:	InChI=1S/C12H9F6NO3/c13-11(14,15)9(20)19-6-8(7-4-2-1-3-5-7)22-10(21)12(16,17)18/
InchiKey:	GLBDCZYKIWFIDR-UHFFFAOYSA-N
Formula:	C12H9F6NO3
SMILES:	O=C(NCC(OC(=O)C(F)(F)F)c1ccccc1)C(F)(F)F
Mol. weight [g/mol]:	329.20
CAS:	13230-75-6

Physical Properties

Property code	Value	Unit	Source
gf	-1276.50	kJ/mol	Joback Method
hf	-1557.83	kJ/mol	Joback Method
hfus	30.49	kJ/mol	Joback Method
hvap	59.04	kJ/mol	Joback Method
log10ws	-3.56		Crippen Method
logp	2.512		Crippen Method
mcvol	185.790	ml/mol	McGowan Method
pc	2181.56	kPa	Joback Method
rinpol	1330.00		NIST Webbook
rinpol	1330.00		NIST Webbook
tb	669.69	K	Joback Method
tc	857.63	K	Joback Method
tf	419.55	K	Joback Method
vc	0.745	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	517.80	J/molxK	669.69	Joback Method
cpg	528.91	J/molxK	701.01	Joback Method
cpg	539.16	J/molxK	732.34	Joback Method
cpg	548.62	J/molxK	763.66	Joback Method
cpg	557.32	J/molxK	794.99	Joback Method

cpg	565.32	J/mol×K	826.31	Joback Method
cpg	572.67	J/mol×K	857.63	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C13230756&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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	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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