Phenylpropanolamine, n,o-bis(heptafluorobutyryl) deriv.

Other names: Phenylpropanolamine, HFB
Inchi: InChI=1S/C17H11F14NO3/c1-7(32-10(33)12(18,19)14(22,23)16(26,27)28)9(8-5-3-2-4-6-
InchiKey: BNYQVYZZVBQKLC-UHFFFAOYSA-N
Formula: C17H11F14NO3
SMILES: CC(NC(=O)C(F)(F)C(F)(F)C(F)(F)F)C(OC(=O)C(F)(F)C(F)(F)C(F)(F)F)c1ccccc1
Mol. weight [g/mol]: 543.25

Physical Properties

Property code	Value	Unit	Source
hfus	34.90	kJ/mol	Joback Method
logp	5.441		Crippen Method
mcvol	270.400	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	853.87	J/mol×K	764.89	Joback Method
cpg	864.57	J/mol×K	794.23	Joback Method
cpg	874.37	J/mol×K	823.57	Joback Method
cpg	883.39	J/mol×K	852.91	Joback Method
cpg	891.71	J/mol×K	882.25	Joback Method
cpg	899.43	J/mol×K	911.59	Joback Method
cpg	906.67	J/mol×K	940.93	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U281491&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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