Pseudoephedrine,N,O-bis(heptafluorobutyryl) deriv.

Other names: Pseudoephedrine, HFB
Pseudoephedrine, HFBA
Inchi: InChI=1S/C18H13F14NO3/c1-8(33(2)11(34)13(19,20)15(23,24)17(27,28)29)10(9-6-4-3-5
InchiKey: BCMWTPKOZMDVHA-UHFFFAOYSA-N
Formula: C18H13F14NO3
SMILES: CC(C(OC(=O)C(F)(F)C(F)(F)C(F)(F)F)c1ccccc1)N(C)C(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 557.28

Physical Properties

Property code	Value	Unit	Source
hfus	35.41	kJ/mol	Joback Method
logp	5.784		Crippen Method
mcvol	284.490	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	894.50	J/mol×K	750.04	Joback Method
cpg	906.32	J/mol×K	778.77	Joback Method
cpg	917.19	J/mol×K	807.51	Joback Method
cpg	927.21	J/mol×K	836.24	Joback Method
cpg	936.47	J/mol×K	864.98	Joback Method
cpg	945.08	J/mol×K	893.71	Joback Method
cpg	953.13	J/mol×K	922.45	Joback Method

Sources

Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?Str2File=U281487
Joback Method: https://en.wikipedia.org/wiki/Joback_method

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

Legend

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