Alprenolol, N,O-di(heptafluorobutyryl)-

Inchi: InChI=1S/C23H21F14NO4/c1-4-7-13-8-5-6-9-15(13)41-11-14(42-17(40)19(26,27)21(30,3
InchiKey: DBANNUCXAQOZMF-UHFFFAOYSA-N
Formula: C23H21F14NO4
SMILES: C=CCc1ccccc1OCC(CN(C(=O)C(F)(F)C(F)(F)C(F)(F)F)C(C)C)OC(=O)C(F)(F)C(F)(F)C(F
Mol. weight [g/mol]: 641.40

Physical Properties

Property code	Value	Unit	Source
hfus	47.88	kJ/mol	Joback Method
log10ws	-7.81		Cheméo Relay (1.0)
logp	6.609		Crippen Method
mcvol	356.510	ml/mol	McGowan Method
rinpol	1861.00		NIST Webbook
rinpol	1861.00		NIST Webbook
tf	335.56	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1176.87	J/mol×K	888.52	Joback Method
cpg	1190.17	J/mol×K	922.14	Joback Method
cpg	1202.58	J/mol×K	955.76	Joback Method
cpg	1214.23	J/mol×K	989.39	Joback Method
cpg	1225.30	J/mol×K	1023.01	Joback Method
cpg	1235.94	J/mol×K	1056.63	Joback Method
cpg	1246.32	J/mol×K	1090.25	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C959084083&Units=SI
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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point