

5-O-benzoyl-n-benzyl-2,3-o-(1-methylethylidene)-r

Inchi:	InChI=1S/C24H24F3NO6/c1-23(2)33-18-17(14-31-21(29)16-11-7-4-8-12-16)32-20(19(18
InchiKey:	DFKBXQZDLXQYPZ-UHFFFAOYSA-N
Formula:	C24H24F3NO6
SMILES:	CC1(C)OC2C(COC(=O)c3ccccc3)OC(N(Cc3ccccc3)C(=O)C(F)(F)F)C2O1
Mol. weight [g/mol]:	479.45

Physical Properties

Property code	Value	Unit	Source
gf	-647.31	kJ/mol	Joback Method
hf	-1261.06	kJ/mol	Joback Method
hfus	68.15	kJ/mol	Joback Method
hvap	99.39	kJ/mol	Joback Method
log10ws	-5.62		Crippen Method
logp	3.679		Crippen Method
mcvol	321.690	ml/mol	McGowan Method
pc	1434.80	kPa	Joback Method
tb	1028.16	K	Joback Method
tc	1267.21	K	Joback Method
tf	691.56	K	Joback Method
vc	1.210	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1140.32	J/molxK	1028.16	Joback Method
cpg	1159.66	J/molxK	1068.00	Joback Method
cpg	1179.18	J/molxK	1107.84	Joback Method
cpg	1199.15	J/molxK	1147.68	Joback Method
cpg	1219.82	J/molxK	1187.52	Joback Method
cpg	1241.48	J/molxK	1227.36	Joback Method
cpg	1264.39	J/molxK	1267.21	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=B6009234&Units=SI
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

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
hvap:	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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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