3,3,5-Trimethylcyclohexyl 2-(pentafluoropropionyloxy)benzoate

Other names: Benzoic acid, 2-pentafluoropropionyloxy-, 3,3,5-trimethylcyclohexyl ester
Heliophan pentafluoropropionate

Inchi: InChI=1S/C19H21F5O4/c1-11-8-12(10-17(2,3)9-11)27-15(25)13-6-4-5-7-14(13)28-16(26

InchiKey: ODDCCKALFXEQNJ-UHFFFAOYSA-N

Formula: C19H21F5O4

SMILES: CC1CC(OC(=O)c2ccccc2OC(=O)C(F)(F)C(F)(F)F)CC(C)(C)C1

Mol. weight [g/mol]: 408.36

Physical Properties

Property code	Value	Unit	Source
gf	-1220.79	kJ/mol	Joback Method
hf	-1669.20	kJ/mol	Joback Method
hfus	32.44	kJ/mol	Joback Method
hvap	71.12	kJ/mol	Joback Method
log10ws	-6.29		Crippen Method
logp	5.161		Crippen Method
mcvol	267.680	ml/mol	McGowan Method
pc	1438.07	kPa	Joback Method
rinpol	1835.00		NIST Webbook
rinpol	1835.00		NIST Webbook
tb	818.70	K	Joback Method
tc	1027.58	K	Joback Method
tf	517.74	K	Joback Method
vc	1.036	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	856.72	J/mol×K	818.70	Joback Method
cpg	873.56	J/mol×K	853.51	Joback Method
cpg	889.59	J/mol×K	888.33	Joback Method
cpg	904.93	J/mol×K	923.14	Joback Method
cpg	919.73	J/mol×K	957.95	Joback Method
cpg	934.10	J/mol×K	992.77	Joback Method

cpg	948.17	J/mol×K	1027.58	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=U373294&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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume