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

Other names: Heliophan heptafluorobutyrate

Benzoic acid, 2-(heptafluorobutyryloxy)-, 3,3,5-trimethylcyclohexyl ester

Inchi: InChI=1S/C20H21F7O4/c1-11-8-12(10-17(2,3)9-11)30-15(28)13-6-4-5-7-14(13)31-16(29

InchiKey: SGFABSORPRSFLG-UHFFFAOYSA-N

Formula: C20H21F7O4

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

Mol. weight [g/mol]: 458.37

Physical Properties

Property code	Value	Unit	Source
gf	-1599.15	kJ/mol	Joback Method
hf	-2090.81	kJ/mol	Joback Method
hfus	33.78	kJ/mol	Joback Method
hvap	70.42	kJ/mol	Joback Method
log10ws	-7.03		Crippen Method
logp	5.796		Crippen Method
mcvol	285.310	ml/mol	McGowan Method
pc	1271.87	kPa	Joback Method
rinpol	1864.00		NIST Webbook
rinpol	1864.00		NIST Webbook
tb	836.89	K	Joback Method
tc	1040.80	K	Joback Method
tf	532.61	K	Joback Method
vc	1.117	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	931.25	J/mol×K	836.89	Joback Method
cpg	947.60	J/mol×K	870.88	Joback Method
cpg	963.22	J/mol×K	904.86	Joback Method
cpg	978.25	J/mol×K	938.85	Joback Method
cpg	992.82	J/mol×K	972.83	Joback Method
cpg	1007.08	J/mol×K	1006.82	Joback Method

cpg	1021.18	J/mol×K	1040.80	Joback Method

Sources

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=U373295&Units=SI
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
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