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

Inchi: InChI=1S/C18H21F3O4/c1-11-8-12(10-17(2,3)9-11)24-15(22)13-6-4-5-7-14(13)25-16(23
InchiKey: PVJSRYNUQOGADZ-UHFFFAOYSA-N
Formula: C18H21F3O4
SMILES: CC1CC(OC(=O)c2ccccc2OC(=O)C(F)(F)F)CC(C)(C)C1
Mol. weight [g/mol]: 358.35

Physical Properties

Property code	Value	Unit	Source
gf	-842.43	kJ/mol	Joback Method
hf	-1247.59	kJ/mol	Joback Method
hfus	31.11	kJ/mol	Joback Method
hvap	71.83	kJ/mol	Joback Method
log10ws	-5.56		Crippen Method
logp	4.526		Crippen Method
mcvol	250.050	ml/mol	McGowan Method
pc	1639.10	kPa	Joback Method
rinpol	1838.00		NIST Webbook
tb	800.51	K	Joback Method
tc	1016.26	K	Joback Method
tf	502.87	K	Joback Method
vc	0.956	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	782.35	J/mol×K	800.51	Joback Method
cpg	799.81	J/mol×K	836.47	Joback Method
cpg	816.39	J/mol×K	872.43	Joback Method
cpg	832.20	J/mol×K	908.39	Joback Method
cpg	847.37	J/mol×K	944.34	Joback Method
cpg	862.01	J/mol×K	980.30	Joback Method
cpg	876.23	J/mol×K	1016.26	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373293&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume