Methyl 3-pentafluoropropionyloxybenzoate

Inchi: InChI=1S/C11H7F5O4/c1-19-8(17)6-3-2-4-7(5-6)20-9(18)10(12,13)11(14,15)16/h2-5H,1
InchiKey: BLTFNURQWJACFJ-UHFFFAOYSA-N
Formula: C11H7F5O4
SMILES: COC(=O)c1cccc(OC(=O)C(F)(F)C(F)(F)F)c1
Mol. weight [g/mol]: 298.16

Physical Properties

Property code	Value	Unit	Source
gf	-1291.69	kJ/mol	Joback Method
hf	-1532.96	kJ/mol	Joback Method
hfus	24.04	kJ/mol	Joback Method
hvap	54.65	kJ/mol	Joback Method
log10ws	-3.42		Crippen Method
logp	2.576		Crippen Method
mcvol	165.820	ml/mol	McGowan Method
pc	2372.59	kPa	Joback Method
rinpol	1252.00		NIST Webbook
tb	625.21	K	Joback Method
tc	817.70	K	Joback Method
tf	404.78	K	Joback Method
vc	0.659	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	434.49	J/mol×K	625.21	Joback Method
cpg	445.31	J/mol×K	657.29	Joback Method
cpg	455.35	J/mol×K	689.37	Joback Method
cpg	464.64	J/mol×K	721.46	Joback Method
cpg	473.21	J/mol×K	753.54	Joback Method
cpg	481.09	J/mol×K	785.62	Joback Method
cpg	488.33	J/mol×K	817.70	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374622&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

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