Benzoic acid, 3-(pentafluoropropionyloxy)-

Inchi: InChI=1S/C10H5F5O4/c11-9(12,10(13,14)15)8(18)19-6-3-1-2-5(4-6)7(16)17/h1-4H,(H,16
InchiKey: YMSPVHHCPYGTAH-UHFFFAOYSA-N
Formula: C10H5F5O4
SMILES: O=C(O)c1cccc(OC(=O)C(F)(F)C(F)(F)F)c1
Mol. weight [g/mol]: 284.14

Physical Properties

Property code	Value	Unit	Source
gf	-1331.93	kJ/mol	Joback Method
hf	-1532.33	kJ/mol	Joback Method
hfus	24.35	kJ/mol	Joback Method
hvap	66.70	kJ/mol	Joback Method
log10ws	-3.24		Crippen Method
logp	2.488		Crippen Method
mcvol	151.730	ml/mol	McGowan Method
pc	2928.17	kPa	Joback Method
rinpol	1332.00		NIST Webbook
rinpol	1332.00		NIST Webbook
tb	672.09	K	Joback Method
tc	858.93	K	Joback Method
tf	432.10	K	Joback Method
vc	0.605	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	408.90	J/mol×K	672.09	Joback Method
cpg	416.99	J/mol×K	703.23	Joback Method
cpg	424.43	J/mol×K	734.37	Joback Method
cpg	431.26	J/mol×K	765.51	Joback Method
cpg	437.52	J/mol×K	796.65	Joback Method
cpg	443.25	J/mol×K	827.79	Joback Method
cpg	448.49	J/mol×K	858.93	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375034&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