Benzoic acid, 3-(heptafluorobutyryloxy)-

Inchi: InChI=1S/C11H5F7O4/c12-9(13,10(14,15)11(16,17)18)8(21)22-6-3-1-2-5(4-6)7(19)20/h1
InchiKey: QUDWSOPBFCWKGP-UHFFFAOYSA-N
Formula: C11H5F7O4
SMILES: O=C(O)c1cccc(OC(=O)C(F)(F)C(F)(F)C(F)(F)F)c1
Mol. weight [g/mol]: 334.14

Physical Properties

Property code	Value	Unit	Source
gf	-1710.29	kJ/mol	Joback Method
hf	-1953.94	kJ/mol	Joback Method
hfus	25.69	kJ/mol	Joback Method
hvap	65.99	kJ/mol	Joback Method
log10ws	-3.97		Crippen Method
logp	3.123		Crippen Method
mcvol	169.360	ml/mol	McGowan Method
pc	2462.92	kPa	Joback Method
rinpol	1371.00		NIST Webbook
tb	690.28	K	Joback Method
tc	871.19	K	Joback Method
tf	446.97	K	Joback Method
vc	0.685	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	477.05	J/mol×K	690.28	Joback Method
cpg	485.15	J/mol×K	720.43	Joback Method
cpg	492.56	J/mol×K	750.58	Joback Method
cpg	499.34	J/mol×K	780.73	Joback Method
cpg	505.53	J/mol×K	810.88	Joback Method
cpg	511.20	J/mol×K	841.03	Joback Method
cpg	516.39	J/mol×K	871.19	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=U375032&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

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