Benzoic acid, 2,2,3,4,4,4-hexafluorobutyl ester

Inchi: InChI=1S/C11H8F6O2/c12-9(11(15,16)17)10(13,14)6-19-8(18)7-4-2-1-3-5-7/h1-5,9H,6H2
InchiKey: ZIDIPWJNDUQITP-UHFFFAOYSA-N
Formula: C11H8F6O2
SMILES: O=C(OCC(F)(F)C(F)C(F)(F)F)c1ccccc1
Mol. weight [g/mol]: 286.17

Physical Properties

Property code	Value	Unit	Source
gf	-1245.39	kJ/mol	Joback Method
hf	-1478.08	kJ/mol	Joback Method
hfus	21.20	kJ/mol	Joback Method
hvap	43.63	kJ/mol	Joback Method
log10ws	-3.91		Crippen Method
logp	3.379		Crippen Method
mcvol	160.150	ml/mol	McGowan Method
pc	2222.89	kPa	Joback Method
rinpol	1232.00		NIST Webbook
rinpol	1232.00		NIST Webbook
tb	542.77	K	Joback Method
tc	723.01	K	Joback Method
tf	305.69	K	Joback Method
vc	0.647	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	402.77	J/mol×K	542.77	Joback Method
cpg	415.39	J/mol×K	572.81	Joback Method
cpg	427.16	J/mol×K	602.85	Joback Method
cpg	438.10	J/mol×K	632.89	Joback Method
cpg	448.27	J/mol×K	662.93	Joback Method
cpg	457.70	J/mol×K	692.97	Joback Method
cpg	466.44	J/mol×K	723.01	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U368915&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