Benzoic acid, 2,2,3,3,4,4,5,5-octafluoropentyl ester

Inchi: InChI=1S/C12H8F8O2/c13-9(14)11(17,18)12(19,20)10(15,16)6-22-8(21)7-4-2-1-3-5-7/h1

InchiKey: ADLMAOYQCWHQOF-UHFFFAOYSA-N

Formula: C12H8F8O2

SMILES: O=C(OCC(F)(F)C(F)(F)C(F)(F)C(F)F)c1ccccc1

Mol. weight [g/mol]: 336.18

Physical Properties

Property code	Value	Unit	Source
gf	-1623.75	kJ/mol	Joback Method
hf	-1899.69	kJ/mol	Joback Method
hfus	22.54	kJ/mol	Joback Method
hvap	42.93	kJ/mol	Joback Method
log10ws	-4.64		Crippen Method
logp	4.014		Crippen Method
mcvol	177.780	ml/mol	McGowan Method
pc	1910.24	kPa	Joback Method
rinpol	1312.00		NIST Webbook
tb	560.96	K	Joback Method
tc	733.54	K	Joback Method
tf	320.56	K	Joback Method
vc	0.729	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	469.68	J/mol×K	560.96	Joback Method
cpg	482.46	J/mol×K	589.72	Joback Method
cpg	494.31	J/mol×K	618.49	Joback Method
cpg	505.30	J/mol×K	647.25	Joback Method
cpg	515.47	J/mol×K	676.01	Joback Method
cpg	524.87	J/mol×K	704.78	Joback Method
cpg	533.56	J/mol×K	733.54	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360676&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