Benzoic acid, pentafluorophenyl ester

Inchi: InChI=1S/C13H5F5O2/c14-7-8(15)10(17)12(11(18)9(7)16)20-13(19)6-4-2-1-3-5-6/h1-5H
InchiKey: WZPWTXZSQHIABL-UHFFFAOYSA-N
Formula: C13H5F5O2
SMILES: O=C(Oc1c(F)c(F)c(F)c(F)c1F)c1ccccc1
Mol. weight [g/mol]: 288.17

Physical Properties

Property code	Value	Unit	Source
gf	-972.72	kJ/mol	Joback Method
hf	-1121.29	kJ/mol	Joback Method
hfus	33.75	kJ/mol	Joback Method
hvap	57.47	kJ/mol	Joback Method
log10ws	-5.22		Crippen Method
logp	3.601		Crippen Method
mcvol	162.800	ml/mol	McGowan Method
pc	2361.07	kPa	Joback Method
rinpol	1499.00		NIST Webbook
rinpol	1499.00		NIST Webbook
tb	647.74	K	Joback Method
tc	848.49	K	Joback Method
tf	426.82	K	Joback Method
vc	0.661	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	401.74	J/mol×K	647.74	Joback Method
cpg	412.26	J/mol×K	681.20	Joback Method
cpg	422.11	J/mol×K	714.66	Joback Method
cpg	431.33	J/mol×K	748.12	Joback Method
cpg	439.90	J/mol×K	781.58	Joback Method
cpg	447.83	J/mol×K	815.04	Joback Method
cpg	455.14	J/mol×K	848.49	Joback Method

Sources

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=U360679&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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