1-Phenylethyl pentafluorobenzoate

Inchi: InChI=1S/C15H9F5O2/c1-7(8-5-3-2-4-6-8)22-15(21)9-10(16)12(18)14(20)13(19)11(9)17/
InchiKey: OITOYBCUNCDVLW-UHFFFAOYSA-N
Formula: C15H9F5O2
SMILES: CC(OC(=O)c1c(F)c(F)c(F)c(F)c1F)c1ccccc1
Mol. weight [g/mol]: 316.22

Physical Properties

Property code	Value	Unit	Source
gf	-958.32	kJ/mol	Joback Method
hf	-1167.85	kJ/mol	Joback Method
hfus	35.41	kJ/mol	Joback Method
hvap	61.53	kJ/mol	Joback Method
log10ws	-5.86		Crippen Method
logp	4.300		Crippen Method
mcvol	190.980	ml/mol	McGowan Method
pc	1989.43	kPa	Joback Method
rinpol	1605.00		NIST Webbook
rinpol	1603.00		NIST Webbook
rinpol	1593.00		NIST Webbook
rinpol	1593.00		NIST Webbook
rinpol	1594.00		NIST Webbook
rinpol	1594.00		NIST Webbook
rinpol	1601.00		NIST Webbook
rinpol	1597.00		NIST Webbook
ripol	2130.00		NIST Webbook
ripol	2118.00		NIST Webbook
ripol	2118.00		NIST Webbook
ripol	2118.00		NIST Webbook
ripol	2170.00		NIST Webbook
ripol	2149.00		NIST Webbook
ripol	2130.00		NIST Webbook
tb	693.06	K	Joback Method
tc	892.47	K	Joback Method
tf	434.36	K	Joback Method
vc	0.767	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	502.07	J/mol×K	693.06	Joback Method
cpg	514.03	J/mol×K	726.29	Joback Method
cpg	525.23	J/mol×K	759.53	Joback Method
cpg	535.66	J/mol×K	792.76	Joback Method
cpg	545.34	J/mol×K	826.00	Joback Method
cpg	554.29	J/mol×K	859.23	Joback Method
cpg	562.52	J/mol×K	892.47	Joback Method

Sources

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=R35004&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume