2-Phenylethyl pentafluorobenzoate

Other names: Benzoic acid, pentafluoro, 2-phenylethyl ester
Inchi: InChI=1S/C15H9F5O2/c16-10-9(11(17)13(19)14(20)12(10)18)15(21)22-7-6-8-4-2-1-3-5-8
InchiKey: ZGQUWVXUEJTWJW-UHFFFAOYSA-N
Formula: C15H9F5O2
SMILES: O=C(OCCc1ccccc1)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 316.22

Physical Properties

Property code	Value	Unit	Source
gf	-955.88	kJ/mol	Joback Method
hf	-1162.57	kJ/mol	Joback Method
hfus	38.93	kJ/mol	Joback Method
hvap	61.92	kJ/mol	Joback Method
log10ws	-5.41		Crippen Method
logp	3.782		Crippen Method
mcvol	190.980	ml/mol	McGowan Method
pc	1975.31	kPa	Joback Method
rinpol	1666.00		NIST Webbook
rinpol	1662.00		NIST Webbook
rinpol	1675.00		NIST Webbook
rinpol	1666.00		NIST Webbook
rinpol	1662.00		NIST Webbook
rinpol	1667.00		NIST Webbook
rinpol	1674.00		NIST Webbook
rinpol	1674.00		NIST Webbook
rinpol	1680.00		NIST Webbook
ripol	2252.00		NIST Webbook
ripol	2259.00		NIST Webbook
ripol	2255.00		NIST Webbook
ripol	2252.00		NIST Webbook
ripol	2259.00		NIST Webbook
ripol	2265.00		NIST Webbook
ripol	2271.00		NIST Webbook
ripol	2276.00		NIST Webbook
ripol	2265.00		NIST Webbook
tb	693.50	K	Joback Method
tc	889.74	K	Joback Method

tf	449.36	K	Joback Method
vc	0.773	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	501.51	J/mol×K	693.50	Joback Method
cpg	513.26	J/mol×K	726.21	Joback Method
cpg	524.28	J/mol×K	758.91	Joback Method
cpg	534.56	J/mol×K	791.62	Joback Method
cpg	544.13	J/mol×K	824.33	Joback Method
cpg	553.00	J/mol×K	857.03	Joback Method
cpg	561.17	J/mol×K	889.74	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R34945&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
ripol: Polar retention indices

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