3-Phenylpropionic acid, pentafluorophenyl ester

Inchi: InChI=1S/C15H9F5O2/c16-10-11(17)13(19)15(14(20)12(10)18)22-9(21)7-6-8-4-2-1-3-5-8

InchiKey: MPTBVJWRSCFIGU-UHFFFAOYSA-N

Formula: C15H9F5O2

SMILES: O=C(CCc1ccccc1)Oc1c(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	-5.48		Crippen Method
logp	3.920		Crippen Method
mcvol	190.980	ml/mol	McGowan Method
pc	1975.31	kPa	Joback Method
rinpol	1704.00		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

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354737&Units=SI

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

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