4-Methylbenzoic acid, pentafluorophenyl ester

Inchi: InChI=1S/C14H7F5O2/c1-6-2-4-7(5-3-6)14(20)21-13-11(18)9(16)8(15)10(17)12(13)19/h2
InchiKey: VIUKYPVYPARUMI-UHFFFAOYSA-N
Formula: C14H7F5O2
SMILES: Cc1ccc(C(=O)Oc2c(F)c(F)c(F)c(F)c2F)cc1
Mol. weight [g/mol]: 302.20

Physical Properties

Property code	Value	Unit	Source
gf	-973.93	kJ/mol	Joback Method
hf	-1153.40	kJ/mol	Joback Method
hfus	35.95	kJ/mol	Joback Method
hvap	60.35	kJ/mol	Joback Method
log10ws	-5.69		Crippen Method
logp	3.910		Crippen Method
mcvol	176.890	ml/mol	McGowan Method
pc	2125.60	kPa	Joback Method
rinpol	1627.00		NIST Webbook
tb	675.60	K	Joback Method
tc	874.76	K	Joback Method
tf	450.61	K	Joback Method
vc	0.718	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	449.69	J/mol×K	675.60	Joback Method
cpg	460.72	J/mol×K	708.79	Joback Method
cpg	471.08	J/mol×K	741.99	Joback Method
cpg	480.77	J/mol×K	775.18	Joback Method
cpg	489.80	J/mol×K	808.37	Joback Method
cpg	498.17	J/mol×K	841.57	Joback Method
cpg	505.88	J/mol×K	874.76	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354151&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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