4-Methylphenol, pentafluoropropionate

Inchi: InChI=1S/C10H7F5O2/c1-6-2-4-7(5-3-6)17-8(16)9(11,12)10(13,14)15/h2-5H,1H3
InchiKey: IJLZCCFDKNCXTR-UHFFFAOYSA-N
Formula: C10H7F5O2
SMILES: Cc1ccc(OC(=O)C(F)(F)C(F)(F)F)cc1
Mol. weight [g/mol]: 254.15

Physical Properties

Property code	Value	Unit	Source
gf	-1066.19	kJ/mol	Joback Method
hf	-1267.52	kJ/mol	Joback Method
hfus	18.67	kJ/mol	Joback Method
hvap	43.27	kJ/mol	Joback Method
log10ws	-3.66		Crippen Method
logp	3.098		Crippen Method
mcvol	144.290	ml/mol	McGowan Method
pc	2492.52	kPa	Joback Method
rinpol	994.00		NIST Webbook
rinpol	994.00		NIST Webbook
tb	526.04	K	Joback Method
tc	714.20	K	Joback Method
tf	321.35	K	Joback Method
vc	0.580	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	348.50	J/mol×K	526.04	Joback Method
cpg	360.42	J/mol×K	557.40	Joback Method
cpg	371.51	J/mol×K	588.76	Joback Method
cpg	381.82	J/mol×K	620.12	Joback Method
cpg	391.39	J/mol×K	651.48	Joback Method
cpg	400.25	J/mol×K	682.84	Joback Method
cpg	408.45	J/mol×K	714.20	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=U375763&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume