4-Methoxyphenol, pentafluoropropionate

Inchi: InChI=1S/C10H7F5O3/c1-17-6-2-4-7(5-3-6)18-8(16)9(11,12)10(13,14)15/h2-5H,1H3
InchiKey: HOWQSLIRYRRFQI-UHFFFAOYSA-N
Formula: C10H7F5O3
SMILES: COc1ccc(OC(=O)C(F)(F)C(F)(F)F)cc1
Mol. weight [g/mol]: 270.15
CAS: 545338-93-0

Physical Properties

Property code	Value	Unit	Source
gf	-1171.19	kJ/mol	Joback Method
hf	-1399.74	kJ/mol	Joback Method
hfus	19.86	kJ/mol	Joback Method
hvap	45.68	kJ/mol	Joback Method
log10ws	-3.30		Crippen Method
logp	2.798		Crippen Method
mcvol	150.160	ml/mol	McGowan Method
pc	2450.74	kPa	Joback Method
rinpol	1130.00		NIST Webbook
rinpol	1130.00		NIST Webbook
tb	548.46	K	Joback Method
tc	735.41	K	Joback Method
tf	343.58	K	Joback Method
vc	0.598	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	372.29	J/mol×K	548.46	Joback Method
cpg	383.85	J/mol×K	579.62	Joback Method
cpg	394.65	J/mol×K	610.78	Joback Method
cpg	404.73	J/mol×K	641.94	Joback Method
cpg	414.11	J/mol×K	673.10	Joback Method
cpg	422.82	J/mol×K	704.26	Joback Method
cpg	430.90	J/mol×K	735.41	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C545338930&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