Pentafluorobenzoic acid, 2,3-dimethylphenyl ester

Other names: 2,3-Dimethylphenol, pentafluorobenzoyl ester
Inchi: InChI=1S/C15H9F5O2/c1-6-4-3-5-8(7(6)2)22-15(21)9-10(16)12(18)14(20)13(19)11(9)17/
InchiKey: AFSWCWLWXSWWLK-UHFFFAOYSA-N
Formula: C15H9F5O2
SMILES: Cc1cccc(OC(=O)c2c(F)c(F)c(F)c(F)c2F)c1C
Mol. weight [g/mol]: 316.22

Physical Properties

Property code	Value	Unit	Source
gf	-975.14	kJ/mol	Joback Method
hf	-1185.51	kJ/mol	Joback Method
hfus	38.15	kJ/mol	Joback Method
hvap	63.24	kJ/mol	Joback Method
log10ws	-6.17		Crippen Method
logp	4.218		Crippen Method
mcvol	190.980	ml/mol	McGowan Method
pc	1923.67	kPa	Joback Method
rinpol	1702.00		NIST Webbook
rinpol	1680.00		NIST Webbook
rinpol	1682.30		NIST Webbook
rinpol	1687.70		NIST Webbook
tb	703.46	K	Joback Method
tc	901.36	K	Joback Method
tf	474.40	K	Joback Method
vc	0.773	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	499.10	J/mol×K	703.46	Joback Method
cpg	510.61	J/mol×K	736.44	Joback Method
cpg	521.42	J/mol×K	769.43	Joback Method
cpg	531.54	J/mol×K	802.41	Joback Method
cpg	540.97	J/mol×K	835.40	Joback Method

cpg	549.70	J/mol×K	868.38	Joback Method
cpg	557.75	J/mol×K	901.36	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360629&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