

5-Isopropyl-2-methylphenyl 2,3,4,5,6-pentafluorobenzoate

Inchi:	InChI=1S/C17H13F5O2/c1-7(2)9-5-4-8(3)10(6-9)24-17(23)11-12(18)14(20)16(22)15(21)
InchiKey:	ZOXDMMLFONUGHZ-UHFFFAOYSA-N
Formula:	C17H13F5O2
SMILES:	<chem>Cc1ccc(C(C)C)cc1OC(=O)c1c(F)c(F)c(F)c(F)c1F</chem>
Mol. weight [g/mol]:	344.28

Physical Properties

Property code	Value	Unit	Source
gf	-960.74	kJ/mol	Joback Method
hf	-1232.07	kJ/mol	Joback Method
hfus	39.81	kJ/mol	Joback Method
hvap	67.30	kJ/mol	Joback Method
log10ws	-6.88		Crippen Method
logp	5.033		Crippen Method
mcvol	219.160	ml/mol	McGowan Method
pc	1647.09	kPa	Joback Method
rinpol	1789.20		NIST Webbook
rinpol	1790.00		NIST Webbook
rinpol	1790.00		NIST Webbook
rinpol	1789.20		NIST Webbook
rinpol	1789.20		NIST Webbook
rinpol	1789.60		NIST Webbook
tb	748.78	K	Joback Method
tc	946.45	K	Joback Method
tf	481.94	K	Joback Method
vc	0.879	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	604.92	J/molxK	748.78	Joback Method
cpg	617.62	J/molxK	781.73	Joback Method
cpg	629.50	J/molxK	814.67	Joback Method
cpg	640.57	J/molxK	847.62	Joback Method

cpg	650.84	J/mol×K	880.56	Joback Method
cpg	660.31	J/mol×K	913.51	Joback Method
cpg	669.00	J/mol×K	946.45	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U378294&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
hvp:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mvol:	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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