Pentafluorobenzoic acid, isopropyl ester

Other names:	Isopropyl 2,3,4,5,6-pentafluorobenzoate
	Methylethyl pentafluorobenzoate
Inchi:	InChI=1S/C10H7F5O2/c1-3(2)17-10(16)4-5(11)7(13)9(15)8(14)6(4)12/h3H,1-2H3
InchiKey:	CHCGOIDAVLLILM-UHFFFAOYSA-N
Formula:	C10H7F5O2
SMILES:	CC(C)OC(=O)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]:	254.15
CAS:	41657-67-4

Physical Properties

Property code	Value	Unit	Source
gf	-1112.83	kJ/mol	Joback Method
hf	-1301.18	kJ/mol	Joback Method
hfus	28.42	kJ/mol	Joback Method
hvap	48.12	kJ/mol	Joback Method
log10ws	-4.32		Crippen Method
logp	2.947		Crippen Method
mcvol	144.290	ml/mol	McGowan Method
pc	2282.77	kPa	Joback Method
rinpol	1100.00		NIST Webbook
rinpol	1063.00		NIST Webbook
rinpol	1085.00		NIST Webbook
rinpol	1068.00		NIST Webbook
rinpol	1070.00		NIST Webbook
rinpol	1100.00		NIST Webbook
ripol	1288.00		NIST Webbook
ripol	1326.00		NIST Webbook
ripol	1330.00		NIST Webbook
ripol	1330.00		NIST Webbook
ripol	1358.00		NIST Webbook
ripol	1358.00		NIST Webbook
tb	551.98	K	Joback Method
tc	727.88	K	Joback Method
tf	351.59	K	Joback Method
vc	0.596	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	340.29	J/mol×K	551.98	Joback Method
cpg	349.97	J/mol×K	581.30	Joback Method
cpg	359.27	J/mol×K	610.61	Joback Method
cpg	368.18	J/mol×K	639.93	Joback Method
cpg	376.71	J/mol×K	669.25	Joback Method
cpg	384.85	J/mol×K	698.56	Joback Method
cpg	392.60	J/mol×K	727.88	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=C41657674&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume