Pentafluorobenzoic acid, 2-butyl ester

Other names: 1-methylpropyl pentafluorobenzoate
Inchi: InChI=1S/C11H9F5O2/c1-3-4(2)18-11(17)5-6(12)8(14)10(16)9(15)7(5)13/h4H,3H2,1-2H3
InchiKey: NYBFFHZPCUJMMG-UHFFFAOYSA-N
Formula: C11H9F5O2
SMILES: CCC(C)OC(=O)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 268.18
CAS: 99483-12-2

Physical Properties

Property code	Value	Unit	Source
gf	-1104.41	kJ/mol	Joback Method
hf	-1321.82	kJ/mol	Joback Method
hfus	31.01	kJ/mol	Joback Method
hvap	50.35	kJ/mol	Joback Method
log10ws	-4.74		Crippen Method
logp	3.337		Crippen Method
mcvol	158.380	ml/mol	McGowan Method
pc	2086.93	kPa	Joback Method
rinpol	1170.00		NIST Webbook
rinpol	1171.00		NIST Webbook
rinpol	1170.00		NIST Webbook
rinpol	1177.00		NIST Webbook
rinpol	1165.00		NIST Webbook
rinpol	1171.00		NIST Webbook
ripol	1444.00		NIST Webbook
ripol	1408.00		NIST Webbook
ripol	1444.00		NIST Webbook
ripol	1424.00		NIST Webbook
ripol	1424.00		NIST Webbook
ripol	1421.00		NIST Webbook
tb	574.86	K	Joback Method
tc	749.37	K	Joback Method
tf	362.86	K	Joback Method
vc	0.651	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	385.86	J/mol×K	574.86	Joback Method
cpg	396.43	J/mol×K	603.95	Joback Method
cpg	406.57	J/mol×K	633.03	Joback Method
cpg	416.27	J/mol×K	662.12	Joback Method
cpg	425.54	J/mol×K	691.20	Joback Method
cpg	434.37	J/mol×K	720.29	Joback Method
cpg	442.76	J/mol×K	749.37	Joback Method

Sources

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=C99483122&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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