Pentafluorobenzoic acid, butyl ester

Other names:	Butyl pentafluorobenzoate
Inchi:	InChI=1S/C11H9F5O2/c1-2-3-4-18-11(17)5-6(12)8(14)10(16)9(15)7(5)13/h2-4H2,1H3
InchiKey:	KVNRLNIGKMHACA-UHFFFAOYSA-N
Formula:	C11H9F5O2
SMILES:	CCCCOC(=O)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]:	268.18
CAS:	97649-90-6

Physical Properties

Property code	Value	Unit	Source
gf	-1101.97	kJ/mol	Joback Method
hf	-1316.54	kJ/mol	Joback Method
hfus	34.53	kJ/mol	Joback Method
hvap	50.74	kJ/mol	Joback Method
log10ws	-4.63		Crippen Method
logp	3.339		Crippen Method
mcvol	158.380	ml/mol	McGowan Method
pc	2071.76	kPa	Joback Method
rinpol	1233.00		NIST Webbook
rinpol	1209.00		NIST Webbook
rinpol	1221.00		NIST Webbook
rinpol	1224.00		NIST Webbook
rinpol	1248.00		NIST Webbook
rinpol	1221.00		NIST Webbook
rinpol	1225.00		NIST Webbook
rinpol	1221.00		NIST Webbook
ripol	1519.00		NIST Webbook
ripol	1517.00		NIST Webbook
ripol	1555.00		NIST Webbook
ripol	1524.00		NIST Webbook
ripol	1543.00		NIST Webbook
ripol	1507.00		NIST Webbook
tb	575.30	K	Joback Method
tc	746.83	K	Joback Method
tf	377.86	K	Joback Method
vc	0.657	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	385.46	J/mol×K	575.30	Joback Method
cpg	395.79	J/mol×K	603.89	Joback Method
cpg	405.72	J/mol×K	632.48	Joback Method
cpg	415.24	J/mol×K	661.06	Joback Method
cpg	424.34	J/mol×K	689.65	Joback Method
cpg	433.03	J/mol×K	718.24	Joback Method
cpg	441.30	J/mol×K	746.83	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C97649906&Units=SI

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

Latest version available from:

https://www.chemeo.com/cid/43-156-1/Pentafluorobenzoic-acid-butyl-ester.pdf

Generated by Cheméo on 2024-10-12 06:54:55.262092225 +0000 UTC m=+3296957.899061487.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.