

4-pentenyl pentafluorobenzoate

Inchi:	InChI=1S/C12H9F5O2/c1-2-3-4-5-19-12(18)6-7(13)9(15)11(17)10(16)8(6)14/h2H,1,3-5H
InchiKey:	ZJJKCIXVVJCZLM-UHFFFAOYSA-N
Formula:	C12H9F5O2
SMILES:	C=CCCCOC(=O)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]:	280.19

Physical Properties

Property code	Value	Unit	Source
gf	-1005.71	kJ/mol	Joback Method
hf	-1211.75	kJ/mol	Joback Method
hfus	35.84	kJ/mol	Joback Method
hvap	52.29	kJ/mol	Joback Method
log10ws	-4.90		Crippen Method
logp	3.505		Crippen Method
mcvol	168.170	ml/mol	McGowan Method
pc	1973.55	kPa	Joback Method
ripol	1309.00		NIST Webbook
ripol	1308.00		NIST Webbook
ripol	1312.00		NIST Webbook
ripol	1300.00		NIST Webbook
ripol	1663.00		NIST Webbook
ripol	1663.00		NIST Webbook
ripol	1658.00		NIST Webbook
ripol	1666.00		NIST Webbook
tb	594.86	K	Joback Method
tc	767.98	K	Joback Method
tf	387.37	K	Joback Method
vc	0.695	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	412.09	J/molxK	594.86	Joback Method
cpg	422.63	J/molxK	623.71	Joback Method

cpg	432.71	J/mol×K	652.57	Joback Method
cpg	442.33	J/mol×K	681.42	Joback Method
cpg	451.51	J/mol×K	710.27	Joback Method
cpg	460.23	J/mol×K	739.13	Joback Method
cpg	468.51	J/mol×K	767.98	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R311881&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
rinpola:	Non-polar retention indices
ripola:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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