pentyl pentafluorobenzoate

Inchi: InChI=1S/C12H11F5O2/c1-2-3-4-5-19-12(18)6-7(13)9(15)11(17)10(16)8(6)14/h2-5H2,1H
InchiKey: OWMXFTXURJTYJD-UHFFFAOYSA-N
Formula: C12H11F5O2
SMILES: CCCCCOC(=O)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 282.21

Physical Properties

Property code	Value	Unit	Source
gf	-1093.55	kJ/mol	Joback Method
hf	-1337.18	kJ/mol	Joback Method
hfus	37.12	kJ/mol	Joback Method
hvap	52.96	kJ/mol	Joback Method
log10ws	-5.05		Crippen Method
logp	3.729		Crippen Method
mcvol	172.470	ml/mol	McGowan Method
pc	1901.92	kPa	Joback Method
rinpol	1340.00		NIST Webbook
rinpol	1328.00		NIST Webbook
rinpol	1322.00		NIST Webbook
rinpol	1310.00		NIST Webbook
rinpol	1322.00		NIST Webbook
rinpol	1322.00		NIST Webbook
rinpol	1319.00		NIST Webbook
rinpol	1321.00		NIST Webbook
rinpol	1319.00		NIST Webbook
ripol	1608.00		NIST Webbook
ripol	1632.00		NIST Webbook
ripol	1635.00		NIST Webbook
ripol	1607.00		NIST Webbook
ripol	1632.00		NIST Webbook
ripol	1564.00		NIST Webbook
ripol	1595.00		NIST Webbook
ripol	1611.00		NIST Webbook
ripol	1608.00		NIST Webbook
tb	598.18	K	Joback Method
tc	768.75	K	Joback Method
tf	389.13	K	Joback Method

vc	0.714	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	432.76	J/mol×K	598.18	Joback Method
cpg	443.90	J/mol×K	626.61	Joback Method
cpg	454.59	J/mol×K	655.04	Joback Method
cpg	464.81	J/mol×K	683.47	Joback Method
cpg	474.58	J/mol×K	711.90	Joback Method
cpg	483.89	J/mol×K	740.33	Joback Method
cpg	492.74	J/mol×K	768.75	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=R311965&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