Pentafluorobenzoic acid, 2-methylpentyl ester

Inchi: InChI=1S/C13H13F5O2/c1-3-4-6(2)5-20-13(19)7-8(14)10(16)12(18)11(17)9(7)15/h6H,3-5
InchiKey: CRUFFQDZFSBYKT-UHFFFAOYSA-N
Formula: C13H13F5O2
SMILES: CCCC(C)COC(=O)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 296.23

Physical Properties

Property code	Value	Unit	Source
gf	-1087.57	kJ/mol	Joback Method
hf	-1363.10	kJ/mol	Joback Method
hfus	36.19	kJ/mol	Joback Method
hvap	54.80	kJ/mol	Joback Method
log10ws	-5.22		Crippen Method
logp	3.975		Crippen Method
mcvol	186.560	ml/mol	McGowan Method
pc	1763.93	kPa	Joback Method
rinpol	1398.00		NIST Webbook
rinpol	1398.00		NIST Webbook
tb	620.62	K	Joback Method
tc	793.08	K	Joback Method
tf	385.40	K	Joback Method
vc	0.763	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	482.18	J/mol×K	620.62	Joback Method
cpg	494.27	J/mol×K	649.36	Joback Method
cpg	505.83	J/mol×K	678.11	Joback Method
cpg	516.87	J/mol×K	706.85	Joback Method
cpg	527.39	J/mol×K	735.59	Joback Method
cpg	537.38	J/mol×K	764.34	Joback Method
cpg	546.85	J/mol×K	793.08	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360624&Units=SI
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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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