Pentafluorobenzoic acid, 4-methoxy-2-methylbutyl ester

Inchi: InChI=1S/C13H13F5O3/c1-6(3-4-20-2)5-21-13(19)7-8(14)10(16)12(18)11(17)9(7)15/h6H

InchiKey: TZATVKGFHODXTB-UHFFFAOYSA-N

Formula: C13H13F5O3

SMILES: COCCC(C)COC(=O)c1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 312.23

Physical Properties

Property code	Value	Unit	Source
gf	-1192.57	kJ/mol	Joback Method
hf	-1495.32	kJ/mol	Joback Method
hfus	37.37	kJ/mol	Joback Method
hvap	57.21	kJ/mol	Joback Method
log10ws	-4.31		Crippen Method
logp	3.212		Crippen Method
mcvol	192.430	ml/mol	McGowan Method
pc	1739.01	kPa	Joback Method
rinpol	1509.00		NIST Webbook
tb	643.04	K	Joback Method
tc	815.54	K	Joback Method
tf	407.63	K	Joback Method
vc	0.781	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	507.84	J/mol×K	643.04	Joback Method
cpg	519.86	J/mol×K	671.79	Joback Method
cpg	531.35	J/mol×K	700.54	Joback Method
cpg	542.32	J/mol×K	729.29	Joback Method
cpg	552.74	J/mol×K	758.04	Joback Method
cpg	562.62	J/mol×K	786.79	Joback Method
cpg	571.94	J/mol×K	815.54	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=U360626&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume