3,7-Dimethyloct-6-enyl 2,3,4,5,6-pentafluorobenzoate

Inchi: InChI=1S/C17H19F5O2/c1-9(2)5-4-6-10(3)7-8-24-17(23)11-12(18)14(20)16(22)15(21)13

InchiKey: QDATXLSCTYMETC-UHFFFAOYSA-N

Formula: C17H19F5O2

SMILES: CC(C)=CCCC(C)CCOC(=O)c1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 350.32

Physical Properties

Property code	Value	Unit	Source
gf	-982.22	kJ/mol	Joback Method
hf	-1338.23	kJ/mol	Joback Method
hfus	45.44	kJ/mol	Joback Method
hvap	63.74	kJ/mol	Joback Method
log10ws	-6.75		Crippen Method
logp	5.311		Crippen Method
mcvol	238.620	ml/mol	McGowan Method
pc	1363.65	kPa	Joback Method
rinpol	1765.00		NIST Webbook
rinpol	1765.00		NIST Webbook
tb	716.18	K	Joback Method
tc	894.61	K	Joback Method
tf	411.44	K	Joback Method
vc	0.969	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	669.03	J/mol×K	716.18	Joback Method
cpg	683.03	J/mol×K	745.92	Joback Method
cpg	696.31	J/mol×K	775.66	Joback Method
cpg	708.90	J/mol×K	805.39	Joback Method
cpg	720.80	J/mol×K	835.13	Joback Method
cpg	732.04	J/mol×K	864.87	Joback Method
cpg	742.64	J/mol×K	894.61	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373583&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