Octan-2-yl 2,3,4,5,6-pentafluorobenzoate

Inchi: InChI=1S/C15H17F5O2/c1-3-4-5-6-7-8(2)22-15(21)9-10(16)12(18)14(20)13(19)11(9)17/h
InchiKey: IWYSQBVZHZVYTO-UHFFFAOYSA-N
Formula: C15H17F5O2
SMILES: CCCCCCC(C)OC(=O)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 324.29

Physical Properties

Property code	Value	Unit	Source
gf	-1070.73	kJ/mol	Joback Method
hf	-1404.38	kJ/mol	Joback Method
hfus	41.37	kJ/mol	Joback Method
hvap	59.25	kJ/mol	Joback Method
log10ws	-6.41		Crippen Method
logp	4.898		Crippen Method
mcvol	214.740	ml/mol	McGowan Method
pc	1510.50	kPa	Joback Method
rinpol	1555.00		NIST Webbook
tb	666.38	K	Joback Method
tc	838.10	K	Joback Method
tf	407.94	K	Joback Method
vc	0.875	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	584.70	J/mol×K	666.38	Joback Method
cpg	598.05	J/mol×K	695.00	Joback Method
cpg	610.79	J/mol×K	723.62	Joback Method
cpg	622.91	J/mol×K	752.24	Joback Method
cpg	634.42	J/mol×K	780.86	Joback Method
cpg	645.33	J/mol×K	809.48	Joback Method
cpg	655.64	J/mol×K	838.10	Joback Method

Sources

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=U373598&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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