Pentafluorobenzoic acid, oct-3-en-2-yl ester

Inchi: InChI=1S/C15H15F5O2/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: VBECRBLNWKRCRC-VOTSOKGWSA-N
Formula: C15H15F5O2
SMILES: CCCCC=CC(C)OC(=O)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 322.27

Physical Properties

Property code	Value	Unit	Source
gf	-990.51	kJ/mol	Joback Method
hf	-1287.16	kJ/mol	Joback Method
hfus	41.57	kJ/mol	Joback Method
hvap	59.21	kJ/mol	Joback Method
log10ws	-6.27		Crippen Method
logp	4.674		Crippen Method
mcvol	210.440	ml/mol	McGowan Method
pc	1573.45	kPa	Joback Method
rinpol	1533.00		NIST Webbook
rinpol	1533.00		NIST Webbook
tb	670.54	K	Joback Method
tc	847.25	K	Joback Method
tf	402.86	K	Joback Method
vc	0.856	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	562.52	J/mol×K	670.54	Joback Method
cpg	575.33	J/mol×K	699.99	Joback Method
cpg	587.52	J/mol×K	729.44	Joback Method
cpg	599.09	J/mol×K	758.90	Joback Method
cpg	610.06	J/mol×K	788.35	Joback Method
cpg	620.44	J/mol×K	817.80	Joback Method
cpg	630.24	J/mol×K	847.25	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=U299185&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