(Z)-Non-3-enyl 2,3,4,5,6-pentafluorobenzoate

Inchi: InChI=1S/C16H17F5O2/c1-2-3-4-5-6-7-8-9-23-16(22)10-11(17)13(19)15(21)14(20)12(10
InchiKey: NVRREISCYJROIC-SREVYHEPSA-N
Formula: C16H17F5O2
SMILES: CCCCCC=CCCOC(=O)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 336.30

Physical Properties

Property code	Value	Unit	Source
gf	-979.65	kJ/mol	Joback Method
hf	-1302.52	kJ/mol	Joback Method
hfus	47.68	kJ/mol	Joback Method
hvap	61.82	kJ/mol	Joback Method
log10ws	-6.57		Crippen Method
logp	5.066		Crippen Method
mcvol	224.530	ml/mol	McGowan Method
pc	1451.25	kPa	Joback Method
rinpol	1714.00		NIST Webbook
tb	693.86	K	Joback Method
tc	868.31	K	Joback Method
tf	429.13	K	Joback Method
vc	0.917	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	614.79	J/mol×K	693.86	Joback Method
cpg	627.98	J/mol×K	722.94	Joback Method
cpg	640.52	J/mol×K	752.01	Joback Method
cpg	652.44	J/mol×K	781.09	Joback Method
cpg	663.74	J/mol×K	810.16	Joback Method
cpg	674.43	J/mol×K	839.24	Joback Method
cpg	684.54	J/mol×K	868.31	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373581&Units=SI

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