2,6-Difluorobenzoic acid, oct-3-en-2-yl ester

Other names: 1-Methyl-2-heptenyl 2,6-difluorobenzoate
Inchi: InChI=1S/C15H18F2O2/c1-3-4-5-6-8-11(2)19-15(18)14-12(16)9-7-10-13(14)17/h6-11H,3
InchiKey: AFBRFUZNFBUQNO-SOFGYWHQSA-N
Formula: C15H18F2O2
SMILES: CCCCC=CC(C)OC(=O)c1c(F)cccc1F
Mol. weight [g/mol]: 268.30

Physical Properties

Property code	Value	Unit	Source
gf	-377.19	kJ/mol	Joback Method
hf	-664.42	kJ/mol	Joback Method
hfus	33.49	kJ/mol	Joback Method
hvap	59.68	kJ/mol	Joback Method
log10ws	-5.27		Crippen Method
logp	4.256		Crippen Method
mcvol	205.130	ml/mol	McGowan Method
pc	1824.72	kPa	Joback Method
rinpol	1682.90		NIST Webbook
rinpol	1682.90		NIST Webbook
tb	657.79	K	Joback Method
tc	851.70	K	Joback Method
tf	363.53	K	Joback Method
vc	0.801	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	540.48	J/mol×K	657.79	Joback Method
cpg	555.37	J/mol×K	690.11	Joback Method
cpg	569.42	J/mol×K	722.43	Joback Method
cpg	582.68	J/mol×K	754.74	Joback Method
cpg	595.17	J/mol×K	787.06	Joback Method
cpg	606.92	J/mol×K	819.38	Joback Method
cpg	617.95	J/mol×K	851.70	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292585&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