2,6-Difluorobenzoic acid, 2,7-dimethyloct-7-en-5-yn-4-yl ester

Inchi: InChI=1S/C17H18F2O2/c1-11(2)8-9-13(10-12(3)4)21-17(20)16-14(18)6-5-7-15(16)19/h5

InchiKey: HJVYDGWGOMWMLH-UHFFFAOYSA-N

Formula: C17H18F2O2

SMILES: C=C(C)C#CC(CC(C)C)OC(=O)c1c(F)cccc1F

Mol. weight [g/mol]: 292.32

Physical Properties

Property code	Value	Unit	Source
gf	-160.92	kJ/mol	Joback Method
hf	-440.26	kJ/mol	Joback Method
hfus	35.48	kJ/mol	Joback Method
hvap	65.34	kJ/mol	Joback Method
log10ws	-5.66		Crippen Method
logp	4.116		Crippen Method
mcvol	224.710	ml/mol	McGowan Method
pc	1780.34	kPa	Joback Method
rinpol	1777.80		NIST Webbook
rinpol	1777.80		NIST Webbook
tb	704.51	K	Joback Method
tc	915.28	K	Joback Method
tf	466.53	K	Joback Method
vc	0.872	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	601.69	J/mol×K	704.51	Joback Method
cpg	617.30	J/mol×K	739.64	Joback Method
cpg	631.93	J/mol×K	774.77	Joback Method
cpg	645.62	J/mol×K	809.90	Joback Method
cpg	658.40	J/mol×K	845.03	Joback Method
cpg	670.29	J/mol×K	880.16	Joback Method
cpg	681.33	J/mol×K	915.28	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=U292587&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