2,6-Difluorobenzoic acid, 2,6-dimethylnon-1-en-3-yn-5-yl ester

Inchi: InChI=1S/C18H20F2O2/c1-5-7-13(4)16(11-10-12(2)3)22-18(21)17-14(19)8-6-9-15(17)20

InchiKey: BJEBUIYNTARECX-UHFFFAOYSA-N

Formula: C18H20F2O2

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

Mol. weight [g/mol]: 306.35

Physical Properties

Property code	Value	Unit	Source
gf	-152.50	kJ/mol	Joback Method
hf	-460.90	kJ/mol	Joback Method
hfus	38.07	kJ/mol	Joback Method
hvap	67.57	kJ/mol	Joback Method
log10ws	-6.08		Crippen Method
logp	4.506		Crippen Method
mcvol	238.800	ml/mol	McGowan Method
pc	1644.42	kPa	Joback Method
rinpol	1858.50		NIST Webbook
tb	727.39	K	Joback Method
tc	935.47	K	Joback Method
tf	477.80	K	Joback Method
vc	0.927	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	655.96	J/mol×K	727.39	Joback Method
cpg	671.92	J/mol×K	762.07	Joback Method
cpg	686.88	J/mol×K	796.75	Joback Method
cpg	700.87	J/mol×K	831.43	Joback Method
cpg	713.94	J/mol×K	866.11	Joback Method
cpg	726.10	J/mol×K	900.79	Joback Method
cpg	737.39	J/mol×K	935.47	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292588&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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