2,6-Difluorobenzoic acid, pent-2-en-4-ynyl ester

Inchi: InChI=1S/C12H8F2O2/c1-2-3-4-8-16-12(15)11-9(13)6-5-7-10(11)14/h1,3-7H,8H2/b4-3+

InchiKey: PXUHUXMKEIVSBN-ONEGZZNKSA-N

Formula: C12H8F2O2

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

Mol. weight [g/mol]: 222.19

Physical Properties

Property code	Value	Unit	Source
gf	-176.94	kJ/mol	Joback Method
hf	-305.32	kJ/mol	Joback Method
hfus	32.22	kJ/mol	Joback Method
hvap	53.24	kJ/mol	Joback Method
log10ws	-3.70		Crippen Method
logp	2.311		Crippen Method
mcvol	154.260	ml/mol	McGowan Method
pc	2732.56	kPa	Joback Method
rinpol	1522.20		NIST Webbook
rinpol	1522.20		NIST Webbook
tb	579.71	K	Joback Method
tc	790.32	K	Joback Method
tf	391.69	K	Joback Method
vc	0.602	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	350.06	J/mol×K	579.71	Joback Method
cpg	361.48	J/mol×K	614.81	Joback Method
cpg	372.19	J/mol×K	649.91	Joback Method
cpg	382.23	J/mol×K	685.01	Joback Method
cpg	391.63	J/mol×K	720.11	Joback Method
cpg	400.41	J/mol×K	755.22	Joback Method
cpg	408.61	J/mol×K	790.32	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=U292583&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