2,6-Difluorobenzoic acid, 2-methyloct-5-yn-4-yl ester

Inchi: InChI=1S/C16H18F2O2/c1-4-5-7-12(10-11(2)3)20-16(19)15-13(17)8-6-9-14(15)18/h6,8-9

InchiKey: XMSIREIWTIXZDM-UHFFFAOYSA-N

Formula: C16H18F2O2

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

Mol. weight [g/mol]: 280.31

Physical Properties

Property code	Value	Unit	Source
gf	-248.63	kJ/mol	Joback Method
hf	-535.26	kJ/mol	Joback Method
hfus	35.48	kJ/mol	Joback Method
hvap	63.71	kJ/mol	Joback Method
log10ws	-5.39		Crippen Method
logp	3.950		Crippen Method
mcvol	214.920	ml/mol	McGowan Method
pc	1856.31	kPa	Joback Method
rinpol	1730.60		NIST Webbook
rinpol	1730.60		NIST Webbook
tb	685.07	K	Joback Method
tc	892.11	K	Joback Method
tf	470.98	K	Joback Method
vc	0.834	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	572.27	J/mol×K	685.07	Joback Method
cpg	587.83	J/mol×K	719.58	Joback Method
cpg	602.47	J/mol×K	754.08	Joback Method
cpg	616.21	J/mol×K	788.59	Joback Method
cpg	629.06	J/mol×K	823.10	Joback Method
cpg	641.04	J/mol×K	857.60	Joback Method
cpg	652.19	J/mol×K	892.11	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=U292586&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

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