3-Fluorobenzoic acid, 2-methyloct-5-yn-4-yl ester

Inchi: InChI=1S/C16H19FO2/c1-4-5-9-15(10-12(2)3)19-16(18)13-7-6-8-14(17)11-13/h6-8,11-12

InchiKey: PHEOHVWHKMLHGE-UHFFFAOYSA-N

Formula: C16H19FO2

SMILES: CCC#CC(CC(C)C)OC(=O)c1cccc(F)c1

Mol. weight [g/mol]: 262.32

Physical Properties

Property code	Value	Unit	Source
gf	-44.19	kJ/mol	Joback Method
hf	-327.68	kJ/mol	Joback Method
hfus	32.79	kJ/mol	Joback Method
hvap	63.86	kJ/mol	Joback Method
log10ws	-5.06		Crippen Method
logp	3.811		Crippen Method
mcvol	213.150	ml/mol	McGowan Method
pc	1956.14	kPa	Joback Method
rinpol	1710.60		NIST Webbook
tb	680.82	K	Joback Method
tc	895.79	K	Joback Method
tf	457.87	K	Joback Method
vc	0.816	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	564.99	J/mol×K	680.82	Joback Method
cpg	581.44	J/mol×K	716.65	Joback Method
cpg	596.86	J/mol×K	752.48	Joback Method
cpg	611.29	J/mol×K	788.31	Joback Method
cpg	624.76	J/mol×K	824.14	Joback Method
cpg	637.29	J/mol×K	859.96	Joback Method
cpg	648.90	J/mol×K	895.79	Joback Method

Sources

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=U292605&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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