

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
hfus	32.79	kJ/mol	Joback Method
ie	9.19	eV	Cheméo Relay (1.0)
logp	3.811		Crippen Method
mcvol	213.150	ml/mol	McGowan Method
rinpol	1710.60		NIST Webbook

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

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292605&Units=SI

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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