2-Fluorobenzoic acid, tridec-2-ynyl ester

Inchi: InChI=1S/C20H27FO2/c1-2-3-4-5-6-7-8-9-10-11-14-17-23-20(22)18-15-12-13-16-19(18)2
InchiKey: ZDLMJQNIVYTDCO-UHFFFAOYSA-N
Formula: C20H27FO2
SMILES: CCCCCCCCCCC#CCOC(=O)c1ccccc1F
Mol. weight [g/mol]: 318.43

Physical Properties

Property code	Value	Unit	Source
gf	-5.63	kJ/mol	Joback Method
hf	-399.68	kJ/mol	Joback Method
hfus	50.20	kJ/mol	Joback Method
hvap	73.54	kJ/mol	Joback Method
log10ws	-6.86		Crippen Method
logp	5.517		Crippen Method
mcvol	269.510	ml/mol	McGowan Method
pc	1412.25	kPa	Joback Method
rinpol	2295.00		NIST Webbook
rinpol	2295.00		NIST Webbook
tb	773.22	K	Joback Method
tc	972.76	K	Joback Method
tf	532.95	K	Joback Method
vc	1.052	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	785.93	J/mol×K	773.22	Joback Method
cpg	803.01	J/mol×K	806.48	Joback Method
cpg	819.06	J/mol×K	839.73	Joback Method
cpg	834.12	J/mol×K	872.99	Joback Method
cpg	848.21	J/mol×K	906.25	Joback Method
cpg	861.38	J/mol×K	939.50	Joback Method
cpg	873.65	J/mol×K	972.76	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299170&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

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