3-Trifluoromethylbenzoic acid, hex-4-yn-3-yl ester

Inchi: InChI=1S/C14H13F3O2/c1-3-6-12(4-2)19-13(18)10-7-5-8-11(9-10)14(15,16)17/h5,7-9,12

InchiKey: RBXLPMKFNMAKTG-UHFFFAOYSA-N

Formula: C14H13F3O2

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

Mol. weight [g/mol]: 270.25

Physical Properties

Property code	Value	Unit	Source
gf	-445.37	kJ/mol	Joback Method
hf	-682.09	kJ/mol	Joback Method
hfus	29.88	kJ/mol	Joback Method
hvap	56.87	kJ/mol	Joback Method
log10ws	-4.82		Crippen Method
logp	3.664		Crippen Method
mcvol	188.510	ml/mol	McGowan Method
pc	2167.36	kPa	Joback Method
rinpol	1478.00		NIST Webbook
tb	630.81	K	Joback Method
tc	841.27	K	Joback Method
tf	453.93	K	Joback Method
vc	0.735	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	480.30	J/mol×K	630.81	Joback Method
cpg	494.66	J/mol×K	665.89	Joback Method
cpg	508.06	J/mol×K	700.96	Joback Method
cpg	520.56	J/mol×K	736.04	Joback Method
cpg	532.19	J/mol×K	771.12	Joback Method
cpg	542.99	J/mol×K	806.20	Joback Method
cpg	553.01	J/mol×K	841.27	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=U299322&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