2,3,4-Trifluorobenzoic acid, hex-4-yn-3-yl ester

Inchi: InChI=1S/C13H11F3O2/c1-3-5-8(4-2)18-13(17)9-6-7-10(14)12(16)11(9)15/h6-8H,4H2,1-
InchiKey: GNXAAQHQJHHCOH-UHFFFAOYSA-N
Formula: C13H11F3O2
SMILES: CC#CC(CC)OC(=O)c1ccc(F)c(F)c1F
Mol. weight [g/mol]: 256.22

Physical Properties

Property code	Value	Unit	Source
gf	-475.89	kJ/mol	Joback Method
hf	-675.64	kJ/mol	Joback Method
hfus	33.93	kJ/mol	Joback Method
hvap	57.26	kJ/mol	Joback Method
log10ws	-4.71		Crippen Method
logp	3.063		Crippen Method
mcvol	174.420	ml/mol	McGowan Method
pc	2265.42	kPa	Joback Method
rinpol	1522.70		NIST Webbook
rinpol	1522.70		NIST Webbook
tb	621.12	K	Joback Method
tc	825.25	K	Joback Method
tf	465.28	K	Joback Method
vc	0.690	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	426.07	J/mol×K	621.12	Joback Method
cpg	438.79	J/mol×K	655.14	Joback Method
cpg	450.84	J/mol×K	689.16	Joback Method
cpg	462.22	J/mol×K	723.18	Joback Method
cpg	472.93	J/mol×K	757.21	Joback Method
cpg	482.97	J/mol×K	791.23	Joback Method
cpg	492.36	J/mol×K	825.25	Joback Method

Sources

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=U292554&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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