3-Trifluoromethylbenzoic acid, pent-2-en-4-ynyl ester

Inchi: InChI=1S/C13H9F3O2/c1-2-3-4-8-18-12(17)10-6-5-7-11(9-10)13(14,15)16/h1,3-7,9H,8H2

InchiKey: FJVUIZZYAQJBAJ-UHFFFAOYSA-N

Formula: C13H9F3O2

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

Mol. weight [g/mol]: 254.20

Physical Properties

Property code	Value	Unit	Source
gf	-350.86	kJ/mol	Joback Method
hf	-519.35	kJ/mol	Joback Method
hfus	30.87	kJ/mol	Joback Method
hvap	52.70	kJ/mol	Joback Method
log10ws	-4.14		Crippen Method
logp	3.052		Crippen Method
mcvol	170.120	ml/mol	McGowan Method
pc	2450.74	kPa	Joback Method
rinpol	1451.00		NIST Webbook
rinpol	1451.00		NIST Webbook
tb	593.65	K	Joback Method
tc	802.09	K	Joback Method
tf	393.45	K	Joback Method
vc	0.664	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	409.28	J/mol×K	593.65	Joback Method
cpg	421.76	J/mol×K	628.39	Joback Method
cpg	433.33	J/mol×K	663.13	Joback Method
cpg	444.05	J/mol×K	697.87	Joback Method
cpg	453.98	J/mol×K	732.61	Joback Method
cpg	463.18	J/mol×K	767.35	Joback Method
cpg	471.71	J/mol×K	802.09	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299321&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

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