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

Inchi: InChI=1S/C12H7F3O2/c1-2-3-4-7-17-12(16)8-5-6-9(13)11(15)10(8)14/h1,3-6H,7H2/b4-3
InchiKey: NNNUEGOUIVSAFU-ONEGZZNKSA-N
Formula: C12H7F3O2
SMILES: C#CC=CCOC(=O)c1ccc(F)c(F)c1F
Mol. weight [g/mol]: 240.18

Physical Properties

Property code	Value	Unit	Source
gf	-381.38	kJ/mol	Joback Method
hf	-512.90	kJ/mol	Joback Method
hfus	34.91	kJ/mol	Joback Method
hvap	53.09	kJ/mol	Joback Method
log10ws	-4.03		Crippen Method
logp	2.450		Crippen Method
mcvol	156.030	ml/mol	McGowan Method
pc	2568.89	kPa	Joback Method
rinpol	1505.30		NIST Webbook
rinpol	1505.30		NIST Webbook
tb	583.96	K	Joback Method
tc	785.79	K	Joback Method
tf	404.80	K	Joback Method
vc	0.620	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	357.44	J/mol×K	583.96	Joback Method
cpg	368.05	J/mol×K	617.60	Joback Method
cpg	378.06	J/mol×K	651.24	Joback Method
cpg	387.47	J/mol×K	684.88	Joback Method
cpg	396.31	J/mol×K	718.51	Joback Method
cpg	404.61	J/mol×K	752.15	Joback Method
cpg	412.40	J/mol×K	785.79	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=U292553&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