trans-3-Trifluoromethylcinnamic acid, but-3-yn-2-yl ester

Inchi: InChI=1S/C14H11F3O2/c1-3-10(2)19-13(18)8-7-11-5-4-6-12(9-11)14(15,16)17/h1,4-10H

InchiKey: JJRPBUOSQJTWJN-BQYQJAHWSA-N

Formula: C14H11F3O2

SMILES: C#CC(C)OC(=O)C=Cc1cccc(C(F)(F)F)c1

Mol. weight [g/mol]: 268.23

Physical Properties

Property code	Value	Unit	Source
gf	-344.88	kJ/mol	Joback Method
hf	-545.27	kJ/mol	Joback Method
hfus	29.94	kJ/mol	Joback Method
hvap	54.53	kJ/mol	Joback Method
log10ws	-4.26		Crippen Method
logp	3.284		Crippen Method
mcvol	184.210	ml/mol	McGowan Method
pc	2250.40	kPa	Joback Method
rinpol	1542.00		NIST Webbook
rinpol	1542.00		NIST Webbook
tb	616.09	K	Joback Method
tc	825.39	K	Joback Method
tf	389.72	K	Joback Method
vc	0.715	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	457.84	J/mol×K	616.09	Joback Method
cpg	471.22	J/mol×K	650.97	Joback Method
cpg	483.64	J/mol×K	685.86	Joback Method
cpg	495.17	J/mol×K	720.74	Joback Method
cpg	505.85	J/mol×K	755.62	Joback Method
cpg	515.76	J/mol×K	790.51	Joback Method
cpg	524.96	J/mol×K	825.39	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299411&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