4-(Trifluoromethyl)benzoic acid, but-3-yn-2-yl ester

Inchi: InChI=1S/C12H9F3O2/c1-3-8(2)17-11(16)9-4-6-10(7-5-9)12(13,14)15/h1,4-8H,2H3
InchiKey: BAVOMQHSSVKTEP-UHFFFAOYSA-N
Formula: C12H9F3O2
SMILES: C#CC(C)OC(=O)c1ccc(C(F)(F)F)cc1
Mol. weight [g/mol]: 242.19

Physical Properties

Property code	Value	Unit	Source
gf	-441.94	kJ/mol	Joback Method
hf	-621.21	kJ/mol	Joback Method
hfus	24.55	kJ/mol	Joback Method
hvap	50.12	kJ/mol	Joback Method
log10ws	-3.98		Crippen Method
logp	2.884		Crippen Method
mcvol	160.330	ml/mol	McGowan Method
pc	2581.96	kPa	Joback Method
rinpol	1250.00		NIST Webbook
rinpol	1250.00		NIST Webbook
tb	566.17	K	Joback Method
tc	773.39	K	Joback Method
tf	372.26	K	Joback Method
vc	0.623	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	382.80	J/mol×K	566.17	Joback Method
cpg	395.53	J/mol×K	600.71	Joback Method
cpg	407.38	J/mol×K	635.24	Joback Method
cpg	418.39	J/mol×K	669.78	Joback Method
cpg	428.61	J/mol×K	704.31	Joback Method
cpg	438.08	J/mol×K	738.85	Joback Method
cpg	446.84	J/mol×K	773.39	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299438&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