2-Trifluoromethylbenzoic acid, 2,7-dimethyloct-7-en-5-yn-4-yl ester

Inchi: InChI=1S/C18H19F3O2/c1-12(2)9-10-14(11-13(3)4)23-17(22)15-7-5-6-8-16(15)18(19,20

InchiKey: GISQIEQNVVNMTC-UHFFFAOYSA-N

Formula: C18H19F3O2

SMILES: C=C(C)C#CC(CC(C)C)OC(=O)c1ccccc1C(F)(F)F

Mol. weight [g/mol]: 324.34

Physical Properties

Property code	Value	Unit	Source
gf	-334.84	kJ/mol	Joback Method
hf	-654.29	kJ/mol	Joback Method
hfus	34.13	kJ/mol	Joback Method
hvap	64.80	kJ/mol	Joback Method
log10ws	-6.10		Crippen Method
logp	4.856		Crippen Method
mcvol	240.570	ml/mol	McGowan Method
pc	1629.85	kPa	Joback Method
rinpol	1743.00		NIST Webbook
rinpol	1743.00		NIST Webbook
tb	718.45	K	Joback Method
tc	927.44	K	Joback Method
tf	468.29	K	Joback Method
vc	0.934	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	666.83	J/mol×K	718.45	Joback Method
cpg	682.70	J/mol×K	753.28	Joback Method
cpg	697.49	J/mol×K	788.11	Joback Method
cpg	711.27	J/mol×K	822.95	Joback Method
cpg	724.10	J/mol×K	857.78	Joback Method
cpg	736.03	J/mol×K	892.61	Joback Method
cpg	747.12	J/mol×K	927.44	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=U299406&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