trans-3-Trifluoromethylcinnamic acid, 2,7-dimethyloct-7-en-5-yn-4-yl ester

Inchi: InChI=1S/C20H21F3O2/c1-14(2)8-10-18(12-15(3)4)25-19(24)11-9-16-6-5-7-17(13-16)20

InchiKey: SHHAYAGTYIIKAS-PKNBQFBNSA-N

Formula: C20H21F3O2

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

Mol. weight [g/mol]: 350.37

Physical Properties

Property code	Value	Unit	Source
gf	-237.78	kJ/mol	Joback Method
hf	-578.35	kJ/mol	Joback Method
hfus	39.51	kJ/mol	Joback Method
hvap	69.20	kJ/mol	Joback Method
log10ws	-6.38		Crippen Method
logp	5.256		Crippen Method
mcvol	264.450	ml/mol	McGowan Method
pc	1460.13	kPa	Joback Method
rinpol	2023.00		NIST Webbook
rinpol	2023.00		NIST Webbook
tb	768.37	K	Joback Method
tc	979.33	K	Joback Method
tf	485.75	K	Joback Method
vc	1.026	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	753.18	J/mol×K	768.37	Joback Method
cpg	769.04	J/mol×K	803.53	Joback Method
cpg	783.84	J/mol×K	838.69	Joback Method
cpg	797.66	J/mol×K	873.85	Joback Method
cpg	810.58	J/mol×K	909.01	Joback Method
cpg	822.67	J/mol×K	944.17	Joback Method
cpg	834.02	J/mol×K	979.33	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299416&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