trans-3-Trifluoromethylcinnamic acid, 2-methyloct-5-yn-4-yl ester

Inchi: InChI=1S/C19H21F3O2/c1-4-5-9-17(12-14(2)3)24-18(23)11-10-15-7-6-8-16(13-15)19(20

InchiKey: KOUQIAYYVYVQOJ-ZHACJKMWSA-N

Formula: C19H21F3O2

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

Mol. weight [g/mol]: 338.36

Physical Properties

Property code	Value	Unit	Source
gf	-325.49	kJ/mol	Joback Method
hf	-673.35	kJ/mol	Joback Method
hfus	39.51	kJ/mol	Joback Method
hvap	67.57	kJ/mol	Joback Method
log10ws	-6.11		Crippen Method
logp	5.090		Crippen Method
mcvol	254.660	ml/mol	McGowan Method
pc	1516.39	kPa	Joback Method
rinpol	1976.00		NIST Webbook
rinpol	1976.00		NIST Webbook
tb	748.93	K	Joback Method
tc	956.37	K	Joback Method
tf	490.20	K	Joback Method
vc	0.989	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	723.01	J/mol×K	748.93	Joback Method
cpg	738.95	J/mol×K	783.50	Joback Method
cpg	753.84	J/mol×K	818.08	Joback Method
cpg	767.75	J/mol×K	852.65	Joback Method
cpg	780.75	J/mol×K	887.22	Joback Method
cpg	792.89	J/mol×K	921.80	Joback Method
cpg	804.25	J/mol×K	956.37	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=U299415&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