trans-(3-trifluoromethyl)cinnamin acid, dodec-9-ynyl ester

Inchi: InChI=1S/C22H27F3O2/c1-2-3-4-5-6-7-8-9-10-11-17-27-21(26)16-15-19-13-12-14-20(18

InchiKey: KYDKOUVIBMAFFL-FOCLMDBBSA-N

Formula: C22H27F3O2

SMILES: CCC#CCCCCCCCCOC(=O)/C=C/c1cccc(C(F)(F)F)c1

Mol. weight [g/mol]: 380.45

Physical Properties

Property code	Value	Unit	Source
hfus	54.32	kJ/mol	Joback Method
ie	8.87	eV	Cheméo Relay (1.0)
logp	6.406		Crippen Method
mcvol	296.930	ml/mol	McGowan Method
rinpol	2399.90		NIST Webbook
rinpol	2399.90		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	893.29	J/mol×K	818.45	Joback Method
cpg	909.59	J/mol×K	851.66	Joback Method
cpg	924.90	J/mol×K	884.88	Joback Method
cpg	939.28	J/mol×K	918.09	Joback Method
cpg	952.82	J/mol×K	951.30	Joback Method
cpg	965.57	J/mol×K	984.51	Joback Method
cpg	977.59	J/mol×K	1017.73	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U292265&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices