trans-3-Trifluoromethylcinnamic acid, undec-2-enyl ester

Inchi: InChI=1S/C21H27F3O2/c1-2-3-4-5-6-7-8-9-10-16-26-20(25)15-14-18-12-11-13-19(17-18

InchiKey: WRRAJOZIRTUBBW-ZNGCIPOTSA-N

Formula: C21H27F3O2

SMILES: CCCCCCCCC=CCOC(=O)C=Cc1cccc(C(F)(F)F)c1

Mol. weight [g/mol]: 368.43

Physical Properties

Property code	Value	Unit	Source
gf	-426.35	kJ/mol	Joback Method
hf	-859.15	kJ/mol	Joback Method
hfus	48.81	kJ/mol	Joback Method
hvap	70.60	kJ/mol	Joback Method
log10ws	-7.14		Crippen Method
logp	6.569		Crippen Method
mcvol	287.140	ml/mol	McGowan Method
pc	1202.29	kPa	Joback Method
rinpol	2318.00		NIST Webbook
rinpol	2318.00		NIST Webbook
tb	790.73	K	Joback Method
tc	982.47	K	Joback Method
tf	431.56	K	Joback Method
vc	1.131	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	859.15	J/mol×K	790.73	Joback Method
cpg	875.34	J/mol×K	822.69	Joback Method
cpg	890.60	J/mol×K	854.64	Joback Method
cpg	905.00	J/mol×K	886.60	Joback Method
cpg	918.61	J/mol×K	918.56	Joback Method
cpg	931.50	J/mol×K	950.51	Joback Method
cpg	943.74	J/mol×K	982.47	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299418&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