trans-(3-Trifluoromethyl)cinnamin acid, undecyl ester

Inchi: InChI=1S/C21H29F3O2/c1-2-3-4-5-6-7-8-9-10-16-26-20(25)15-14-18-12-11-13-19(17-18
InchiKey: LKWXCSBKAVHDCK-CCEZHUSRSA-N
Formula: C21H29F3O2
SMILES: CCCCCCCCCCCOC(=O)C=Cc1cccc(C(F)(F)F)c1
Mol. weight [g/mol]: 370.45

Physical Properties

Property code	Value	Unit	Source
gf	-506.57	kJ/mol	Joback Method
hf	-976.37	kJ/mol	Joback Method
hfus	48.61	kJ/mol	Joback Method
hvap	70.64	kJ/mol	Joback Method
log10ws	-7.28		Crippen Method
logp	6.793		Crippen Method
mcvol	291.440	ml/mol	McGowan Method
pc	1160.08	kPa	Joback Method
rinpol	2295.20		NIST Webbook
tb	786.57	K	Joback Method
tc	974.30	K	Joback Method
tf	436.64	K	Joback Method
vc	1.151	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	884.20	J/mol×K	786.57	Joback Method
cpg	900.91	J/mol×K	817.86	Joback Method
cpg	916.64	J/mol×K	849.15	Joback Method
cpg	931.47	J/mol×K	880.43	Joback Method
cpg	945.45	J/mol×K	911.72	Joback Method
cpg	958.63	J/mol×K	943.01	Joback Method
cpg	971.08	J/mol×K	974.30	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=U292264&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