trans-3-(Trifluoromethyl)cinnamic acid, pentadecyl ester

Inchi: InChI=1S/C25H37F3O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-20-30-24(29)19-18-22-16-15

InchiKey: JMWFVIXXKWTWQF-VHEBQXMUSA-N

Formula: C25H37F3O2

SMILES: CCCCCCCCCCCCCCCOC(=O)C=Cc1cccc(C(F)(F)F)c1

Mol. weight [g/mol]: 426.56

Physical Properties

Property code	Value	Unit	Source
gf	-472.89	kJ/mol	Joback Method
hf	-1058.93	kJ/mol	Joback Method
hfus	58.97	kJ/mol	Joback Method
hvap	79.55	kJ/mol	Joback Method
log10ws	-8.96		Crippen Method
logp	8.353		Crippen Method
mcvol	347.800	ml/mol	McGowan Method
pc	907.24	kPa	Joback Method
rinpol	2718.00		NIST Webbook
rinpol	2718.00		NIST Webbook
tb	878.09	K	Joback Method
tc	1075.65	K	Joback Method
tf	481.72	K	Joback Method
vc	1.375	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1124.88	J/mol×K	878.09	Joback Method
cpg	1143.09	J/mol×K	911.02	Joback Method
cpg	1160.22	J/mol×K	943.94	Joback Method
cpg	1176.37	J/mol×K	976.87	Joback Method
cpg	1191.59	J/mol×K	1009.80	Joback Method
cpg	1205.98	J/mol×K	1042.73	Joback Method
cpg	1219.60	J/mol×K	1075.65	Joback Method

Sources

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=U299877&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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