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

Inchi: InChI=1S/C24H35F3O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-19-29-23(28)18-17-21-15-14-16

InchiKey: HWKBCJSJTNQWQD-ISLYRVAYSA-N

Formula: C24H35F3O2

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

Mol. weight [g/mol]: 412.53

Physical Properties

Property code	Value	Unit	Source
gf	-481.31	kJ/mol	Joback Method
hf	-1038.29	kJ/mol	Joback Method
hfus	56.38	kJ/mol	Joback Method
hvap	77.32	kJ/mol	Joback Method
log10ws	-8.54		Crippen Method
logp	7.963		Crippen Method
mcvol	333.710	ml/mol	McGowan Method
pc	962.08	kPa	Joback Method
rinpol	2624.00		NIST Webbook
rinpol	2624.00		NIST Webbook
tb	855.21	K	Joback Method
tc	1049.14	K	Joback Method
tf	470.45	K	Joback Method
vc	1.319	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1063.56	J/mol×K	855.21	Joback Method
cpg	1081.34	J/mol×K	887.53	Joback Method
cpg	1098.08	J/mol×K	919.85	Joback Method
cpg	1113.85	J/mol×K	952.18	Joback Method
cpg	1128.73	J/mol×K	984.50	Joback Method
cpg	1142.78	J/mol×K	1016.82	Joback Method
cpg	1156.07	J/mol×K	1049.14	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=U299876&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