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

Inchi: InChI=1S/C27H41F3O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-22-32-26(31)21-20-24

InchiKey: PJHBINDYCZVCPL-QZQOTICOSA-N

Formula: C27H41F3O2

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

Mol. weight [g/mol]: 454.61

Physical Properties

Property code	Value	Unit	Source
gf	-456.05	kJ/mol	Joback Method
hf	-1100.21	kJ/mol	Joback Method
hfus	64.15	kJ/mol	Joback Method
hvap	84.00	kJ/mol	Joback Method
log10ws	-9.80		Crippen Method
logp	9.133		Crippen Method
mcvol	375.980	ml/mol	McGowan Method
pc	810.76	kPa	Joback Method
rinpol	2706.90		NIST Webbook
rinpol	2706.90		NIST Webbook
tb	923.85	K	Joback Method
tc	1131.41	K	Joback Method
tf	504.26	K	Joback Method
vc	1.486	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1249.51	J/mol×K	923.85	Joback Method
cpg	1268.75	J/mol×K	958.44	Joback Method
cpg	1286.83	J/mol×K	993.04	Joback Method
cpg	1303.85	J/mol×K	1027.63	Joback Method
cpg	1319.90	J/mol×K	1062.22	Joback Method
cpg	1335.09	J/mol×K	1096.81	Joback Method
cpg	1349.49	J/mol×K	1131.41	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292267&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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