trans-(3-Trifluoromethyl)cinnamin acid, 4-hexadecyl ester

Inchi: InChI=1S/C26H39F3O2/c1-3-5-6-7-8-9-10-11-12-13-18-24(15-4-2)31-25(30)20-19-22-16

InchiKey: LBDQLZSHJQWBDI-FMQUCBEESA-N

Formula: C26H39F3O2

SMILES: CCCCCCCCCCCCC(CCC)OC(=O)C=Cc1cccc(C(F)(F)F)c1

Mol. weight [g/mol]: 440.58

Physical Properties

Property code	Value	Unit	Source
gf	-466.91	kJ/mol	Joback Method
hf	-1084.85	kJ/mol	Joback Method
hfus	58.04	kJ/mol	Joback Method
hvap	81.39	kJ/mol	Joback Method
log10ws	-9.49		Crippen Method
logp	8.742		Crippen Method
mcvol	361.890	ml/mol	McGowan Method
pc	861.00	kPa	Joback Method
rinpol	2515.10		NIST Webbook
rinpol	2515.10		NIST Webbook
tb	900.53	K	Joback Method
tc	1102.64	K	Joback Method
tf	477.99	K	Joback Method
vc	1.425	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1187.31	J/mol×K	900.53	Joback Method
cpg	1205.98	J/mol×K	934.22	Joback Method
cpg	1223.53	J/mol×K	967.90	Joback Method
cpg	1240.04	J/mol×K	1001.59	Joback Method
cpg	1255.60	J/mol×K	1035.27	Joback Method
cpg	1270.29	J/mol×K	1068.96	Joback Method
cpg	1284.19	J/mol×K	1102.64	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292266&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