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

Inchi: InChI=1S/C26H39F3O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-21-31-25(30)20-19-23-17

InchiKey: MQBGUHUKOSBORD-FMQUCBEESA-N

Formula: C26H39F3O2

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

Mol. weight [g/mol]: 440.58

Physical Properties

Property code	Value	Unit	Source
gf	-464.47	kJ/mol	Joback Method
hf	-1079.57	kJ/mol	Joback Method
hfus	61.56	kJ/mol	Joback Method
hvap	81.78	kJ/mol	Joback Method
log10ws	-9.38		Crippen Method
logp	8.743		Crippen Method
mcvol	361.890	ml/mol	McGowan Method
pc	856.97	kPa	Joback Method
rinpol	2816.00		NIST Webbook
rinpol	2816.00		NIST Webbook
tb	900.97	K	Joback Method
tc	1103.05	K	Joback Method
tf	492.99	K	Joback Method
vc	1.431	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1186.87	J/mol×K	900.97	Joback Method
cpg	1205.57	J/mol×K	934.65	Joback Method
cpg	1223.15	J/mol×K	968.33	Joback Method
cpg	1239.71	J/mol×K	1002.01	Joback Method
cpg	1255.32	J/mol×K	1035.69	Joback Method
cpg	1270.08	J/mol×K	1069.37	Joback Method
cpg	1284.08	J/mol×K	1103.05	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299878&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