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

Inchi: InChI=1S/C20H27F3O2/c1-2-3-4-5-6-7-8-9-15-25-19(24)14-13-17-11-10-12-18(16-17)20

InchiKey: BVYALUOSXKFCHD-BUHFOSPRSA-N

Formula: C20H27F3O2

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

Mol. weight [g/mol]: 356.42

Physical Properties

Property code	Value	Unit	Source
gf	-514.99	kJ/mol	Joback Method
hf	-955.73	kJ/mol	Joback Method
hfus	46.02	kJ/mol	Joback Method
hvap	68.42	kJ/mol	Joback Method
log10ws	-6.87		Crippen Method
logp	6.403		Crippen Method
mcvol	277.350	ml/mol	McGowan Method
pc	1239.83	kPa	Joback Method
rinpol	2219.00		NIST Webbook
tb	763.69	K	Joback Method
tc	950.71	K	Joback Method
tf	425.37	K	Joback Method
vc	1.095	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	826.13	J/mol×K	763.69	Joback Method
cpg	842.52	J/mol×K	794.86	Joback Method
cpg	857.96	J/mol×K	826.03	Joback Method
cpg	872.50	J/mol×K	857.20	Joback Method
cpg	886.20	J/mol×K	888.37	Joback Method
cpg	899.11	J/mol×K	919.54	Joback Method
cpg	911.30	J/mol×K	950.71	Joback Method

Sources

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=U299873&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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