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

Inchi: InChI=1S/C18H23F3O2/c1-2-3-4-5-6-7-13-23-17(22)12-11-15-9-8-10-16(14-15)18(19,20

InchiKey: PUJCNFSVCZJTQA-VAWYXSNFSA-N

Formula: C18H23F3O2

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

Mol. weight [g/mol]: 328.37

Physical Properties

Property code	Value	Unit	Source
gf	-531.83	kJ/mol	Joback Method
hf	-914.45	kJ/mol	Joback Method
hfus	40.84	kJ/mol	Joback Method
hvap	63.97	kJ/mol	Joback Method
log10ws	-6.03		Crippen Method
logp	5.622		Crippen Method
mcvol	249.170	ml/mol	McGowan Method
pc	1426.15	kPa	Joback Method
rinpol	1926.00		NIST Webbook
tb	717.93	K	Joback Method
tc	905.27	K	Joback Method
tf	402.83	K	Joback Method
vc	0.983	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	712.92	J/mol×K	717.93	Joback Method
cpg	728.68	J/mol×K	749.15	Joback Method
cpg	743.52	J/mol×K	780.38	Joback Method
cpg	757.48	J/mol×K	811.60	Joback Method
cpg	770.62	J/mol×K	842.82	Joback Method
cpg	782.98	J/mol×K	874.04	Joback Method
cpg	794.62	J/mol×K	905.27	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299872&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

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