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

Inchi: InChI=1S/C14H15F3O2/c1-2-3-9-19-13(18)8-7-11-5-4-6-12(10-11)14(15,16)17/h4-8,10H

InchiKey: RDQYFKFIUCPJLN-BQYQJAHWSA-N

Formula: C14H15F3O2

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

Mol. weight [g/mol]: 272.26

Physical Properties

Property code	Value	Unit	Source
gf	-565.51	kJ/mol	Joback Method
hf	-831.89	kJ/mol	Joback Method
hfus	30.48	kJ/mol	Joback Method
hvap	55.06	kJ/mol	Joback Method
log10ws	-4.35		Crippen Method
logp	4.062		Crippen Method
mcvol	192.810	ml/mol	McGowan Method
pc	1950.95	kPa	Joback Method
rinpol	1624.00		NIST Webbook
tb	626.41	K	Joback Method
tc	819.86	K	Joback Method
tf	357.75	K	Joback Method
vc	0.758	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	500.19	J/mol×K	626.41	Joback Method
cpg	514.41	J/mol×K	658.65	Joback Method
cpg	527.75	J/mol×K	690.89	Joback Method
cpg	540.24	J/mol×K	723.14	Joback Method
cpg	551.95	J/mol×K	755.38	Joback Method
cpg	562.90	J/mol×K	787.62	Joback Method
cpg	573.15	J/mol×K	819.86	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299868&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