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

Inchi: InChI=1S/C14H13F3O2/c15-14(16,17)11-4-1-3-10(9-11)7-8-13(18)19-12-5-2-6-12/h1,3-4

InchiKey: XTIPEEJGVMTZBI-BQYQJAHWSA-N

Formula: C14H13F3O2

SMILES: O=C(C=Cc1cccc(C(F)(F)F)c1)OC1CCC1

Mol. weight [g/mol]: 270.25

Physical Properties

Property code	Value	Unit	Source
gf	-516.86	kJ/mol	Joback Method
hf	-765.25	kJ/mol	Joback Method
hfus	26.52	kJ/mol	Joback Method
hvap	55.15	kJ/mol	Joback Method
log10ws	-4.36		Crippen Method
logp	3.814		Crippen Method
mcvol	181.950	ml/mol	McGowan Method
pc	2248.26	kPa	Joback Method
rinpol	1701.00		NIST Webbook
tb	637.42	K	Joback Method
tc	849.79	K	Joback Method
tf	372.17	K	Joback Method
vc	0.708	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	487.20	J/mol×K	637.42	Joback Method
cpg	502.53	J/mol×K	672.82	Joback Method
cpg	516.73	J/mol×K	708.21	Joback Method
cpg	529.89	J/mol×K	743.61	Joback Method
cpg	542.08	J/mol×K	779.00	Joback Method
cpg	553.37	J/mol×K	814.40	Joback Method
cpg	563.86	J/mol×K	849.79	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=U292259&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