Cyclopropanecarboxylic acid, trans-2-phenyl-, 1,1,1-trifluoroprop-2-yl ester

Inchi: InChI=1S/C13H13F3O2/c1-8(13(14,15)16)18-12(17)11-7-10(11)9-5-3-2-4-6-9/h2-6,8,10-

InchiKey: JHAXCIFZEDXPAR-UHFFFAOYSA-N

Formula: C13H13F3O2

SMILES: CC(OC(=O)C1CC1c1ccccc1)C(F)(F)F

Mol. weight [g/mol]: 258.24

Physical Properties

Property code	Value	Unit	Source
gf	-593.92	kJ/mol	Joback Method
hf	-869.82	kJ/mol	Joback Method
hfus	23.76	kJ/mol	Joback Method
hvap	51.43	kJ/mol	Joback Method
log10ws	-3.62		Crippen Method
logp	3.284		Crippen Method
mcvol	172.160	ml/mol	McGowan Method
pc	2267.57	kPa	Joback Method
rinpol	1416.00		NIST Webbook
rinpol	1416.00		NIST Webbook
tb	596.02	K	Joback Method
tc	799.76	K	Joback Method
tf	337.74	K	Joback Method
vc	0.672	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	458.58	J/mol×K	596.02	Joback Method
cpg	474.35	J/mol×K	629.98	Joback Method
cpg	489.03	J/mol×K	663.93	Joback Method
cpg	502.68	J/mol×K	697.89	Joback Method
cpg	515.35	J/mol×K	731.85	Joback Method
cpg	527.12	J/mol×K	765.80	Joback Method
cpg	538.05	J/mol×K	799.76	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=U406832&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