Cyclopropanecarboxylic acid, trans-2-phenyl-, 2,2,3,3-tetrafluoropropyl ester

Inchi: InChI=1S/C13H12F4O2/c14-12(15)13(16,17)7-19-11(18)10-6-9(10)8-4-2-1-3-5-8/h1-5,9-

InchiKey: DXPQVJBVQPBVMP-UHFFFAOYSA-N

Formula: C13H12F4O2

SMILES: O=C(OCC(F)(F)C(F)F)C1CC1c1ccccc1

Mol. weight [g/mol]: 276.23

Physical Properties

Property code	Value	Unit	Source
gf	-788.73	kJ/mol	Joback Method
hf	-1065.93	kJ/mol	Joback Method
hfus	26.84	kJ/mol	Joback Method
hvap	50.62	kJ/mol	Joback Method
log10ws	-3.47		Crippen Method
logp	3.234		Crippen Method
mcvol	173.930	ml/mol	McGowan Method
pc	2173.43	kPa	Joback Method
rinpol	1512.00		NIST Webbook
rinpol	1512.00		NIST Webbook
tb	595.29	K	Joback Method
tc	790.03	K	Joback Method
tf	338.33	K	Joback Method
vc	0.691	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	466.71	J/mol×K	595.29	Joback Method
cpg	481.76	J/mol×K	627.75	Joback Method
cpg	495.80	J/mol×K	660.20	Joback Method
cpg	508.88	J/mol×K	692.66	Joback Method
cpg	521.06	J/mol×K	725.12	Joback Method
cpg	532.39	J/mol×K	757.57	Joback Method
cpg	542.92	J/mol×K	790.03	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406833&Units=SI

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