Cyclopropanecarboxylic acid, trans-2-phenyl-, 2-methyloct-5-en-4-yl ester

Inchi: InChI=1S/C19H24O2/c1-4-5-11-16(12-14(2)3)21-19(20)18-13-17(18)15-9-7-6-8-10-15/h6

InchiKey: PBDQUGCDKHVFOM-UHFFFAOYSA-N

Formula: C19H24O2

SMILES: CCC#CC(CC(C)C)OC(=O)C1CC1c1ccccc1

Mol. weight [g/mol]: 284.39

Physical Properties

Property code	Value	Unit	Source
gf	238.55	kJ/mol	Joback Method
hf	-129.56	kJ/mol	Joback Method
hfus	37.08	kJ/mol	Joback Method
hvap	70.30	kJ/mol	Joback Method
log10ws	-5.02		Crippen Method
logp	4.161		Crippen Method
mcvol	242.790	ml/mol	McGowan Method
pc	1747.74	kPa	Joback Method
rinpol	2074.00		NIST Webbook
tb	747.28	K	Joback Method
tc	973.12	K	Joback Method
tf	492.27	K	Joback Method
vc	0.921	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	710.03	J/mol×K	747.28	Joback Method
cpg	729.04	J/mol×K	784.92	Joback Method
cpg	746.75	J/mol×K	822.56	Joback Method
cpg	763.23	J/mol×K	860.20	Joback Method
cpg	778.56	J/mol×K	897.84	Joback Method
cpg	792.80	J/mol×K	935.48	Joback Method
cpg	806.03	J/mol×K	973.12	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406910&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

Latest version available from:
https://www.chemeo.com/cid/89-499-1/Cyclopropanecarboxylic-acid-trans-2-phenyl-2-methyloct-5-en-4-yl-ester.pdf
Generated by Cheméo on 2024-04-30 16:39:56.090314621 +0000 UTC m=+16784445.010891937.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.