

Cyclopropanecarboxylic acid, trans-2-phenyl-, nonyl ester

Inchi:	InChI=1S/C19H28O2/c1-2-3-4-5-6-7-11-14-21-19(20)18-15-17(18)16-12-9-8-10-13-16/h
InchiKey:	DDSRIPNWUSPZSS-UHFFFAOYSA-N
Formula:	C19H28O2
SMILES:	CCCCCCCCCOC(=O)C1CC1c1ccccc1
Mol. weight [g/mol]:	288.42

Physical Properties

Property code	Value	Unit	Source
gf	40.63	kJ/mol	Joback Method
hf	-391.30	kJ/mol	Joback Method
hfus	41.00	kJ/mol	Joback Method
hvap	68.92	kJ/mol	Joback Method
log10ws	-5.36		Crippen Method
logp	5.084		Crippen Method
mcvol	251.390	ml/mol	McGowan Method
pc	1516.39	kPa	Joback Method
rinpol	2236.00		NIST Webbook
tb	739.16	K	Joback Method
tc	939.23	K	Joback Method
tf	416.17	K	Joback Method
vc	0.972	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	755.58	J/molxK	739.16	Joback Method
cpg	774.28	J/molxK	772.51	Joback Method
cpg	791.87	J/molxK	805.85	Joback Method
cpg	808.40	J/molxK	839.20	Joback Method
cpg	823.92	J/molxK	872.54	Joback Method
cpg	838.49	J/molxK	905.89	Joback Method
cpg	852.16	J/molxK	939.23	Joback Method
dvisc	0.0018304	Paxs	416.17	Joback Method
dvisc	0.0011347	Paxs	470.00	Joback Method

dvisc	0.0007760	Paxs	523.83	Joback Method
dvisc	0.0005697	Paxs	577.66	Joback Method
dvisc	0.0004408	Paxs	631.50	Joback Method
dvisc	0.0003551	Paxs	685.33	Joback Method
dvisc	0.0002952	Paxs	739.16	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406000&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
dvisc:	Dynamic viscosity
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

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