

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

Inchi:	InChI=1S/C15H20O2/c1-2-3-7-10-17-15(16)14-11-13(14)12-8-5-4-6-9-12/h4-6,8-9,13-14
InchiKey:	VRFWRIWWEFJWRH-UHFFFAOYSA-N
Formula:	C15H20O2
SMILES:	CCCCCOC(=O)C1CC1c1ccccc1
Mol. weight [g/mol]:	232.32

Physical Properties

Property code	Value	Unit	Source
gf	6.95	kJ/mol	Joback Method
hf	-308.74	kJ/mol	Joback Method
hfus	30.64	kJ/mol	Joback Method
hvap	60.02	kJ/mol	Joback Method
log10ws	-3.68		Crippen Method
logp	3.523		Crippen Method
mcvol	195.030	ml/mol	McGowan Method
pc	2096.50	kPa	Joback Method
rinpol	1816.00		NIST Webbook
rinpol	1816.00		NIST Webbook
tb	647.64	K	Joback Method
tc	857.63	K	Joback Method
tf	371.09	K	Joback Method
vc	0.748	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	533.93	J/molxK	647.64	Joback Method
cpg	551.66	J/molxK	682.64	Joback Method
cpg	568.29	J/molxK	717.64	Joback Method
cpg	583.88	J/molxK	752.63	Joback Method
cpg	598.46	J/molxK	787.63	Joback Method
cpg	612.11	J/molxK	822.63	Joback Method
cpg	624.86	J/molxK	857.63	Joback Method
dvisc	0.0019670	Paxs	371.09	Joback Method

dvisc	0.0013116	Paxs	417.18	Joback Method
dvisc	0.0009481	Paxs	463.27	Joback Method
dvisc	0.0007268	Paxs	509.37	Joback Method
dvisc	0.0005822	Paxs	555.46	Joback Method
dvisc	0.0004826	Paxs	601.55	Joback Method
dvisc	0.0004108	Paxs	647.64	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405997&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

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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