

Cyclopentanecarboxylic acid, 2-methylphenyl ester

Inchi:	InChI=1S/C13H16O2/c1-10-6-2-5-9-12(10)15-13(14)11-7-3-4-8-11/h2,5-6,9,11H,3-4,7-8H
InchiKey:	UGVXBKWUWXZBOP-UHFFFAOYSA-N
Formula:	C13H16O2
SMILES:	<chem>Cc1ccccc1OC(=O)C1CCCC1</chem>
Mol. weight [g/mol]:	204.26
CAS:	55229-43-1

Physical Properties

Property code	Value	Unit	Source
gf	-36.01	kJ/mol	Joback Method
hf	-270.91	kJ/mol	Joback Method
hfus	19.80	kJ/mol	Joback Method
hvap	56.88	kJ/mol	Joback Method
log10ws	-3.59		Crippen Method
logp	3.091		Crippen Method
mcvol	166.850	ml/mol	McGowan Method
pc	2701.41	kPa	Joback Method
tb	620.07	K	Joback Method
tc	853.14	K	Joback Method
tf	358.27	K	Joback Method
vc	0.621	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	431.75	J/molxK	620.07	Joback Method
cpg	449.72	J/molxK	658.92	Joback Method
cpg	466.46	J/molxK	697.76	Joback Method
cpg	482.00	J/molxK	736.61	Joback Method
cpg	496.40	J/molxK	775.45	Joback Method
cpg	509.69	J/molxK	814.30	Joback Method
cpg	521.92	J/molxK	853.14	Joback Method
dvisc	0.0019305	Paxs	358.27	Joback Method
dvisc	0.0011203	Paxs	401.90	Joback Method

dvisc	0.0007232	Paxs	445.54	Joback Method
dvisc	0.0005048	Paxs	489.17	Joback Method
dvisc	0.0003737	Paxs	532.80	Joback Method
dvisc	0.0002896	Paxs	576.44	Joback Method
dvisc	0.0002326	Paxs	620.07	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=C55229431&Units=SI

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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