3-Cyclopentylpropionic acid, 3-methylphenyl ester

Inchi: InChI=1S/C15H20O2/c1-12-5-4-8-14(11-12)17-15(16)10-9-13-6-2-3-7-13/h4-5,8,11,13H,

InchiKey: OZLLFMAAVPMRQE-UHFFFAOYSA-N

Formula: C15H20O2

SMILES: Cc1cccc(OC(=O)CCC2CCCC2)c1

Mol. weight [g/mol]: 232.32

Physical Properties

Property code	Value	Unit	Source
gf	-19.17	kJ/mol	Joback Method
hf	-312.19	kJ/mol	Joback Method
hfus	24.98	kJ/mol	Joback Method
hvap	61.34	kJ/mol	Joback Method
log10ws	-4.43		Crippen Method
logp	3.871		Crippen Method
mcvol	195.030	ml/mol	McGowan Method
pc	2233.41	kPa	Joback Method
rinpol	1800.00		NIST Webbook
tb	665.83	K	Joback Method
tc	890.08	K	Joback Method
tf	380.81	K	Joback Method
vc	0.733	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	536.27	J/mol×K	665.83	Joback Method
cpg	554.97	J/mol×K	703.20	Joback Method
cpg	572.41	J/mol×K	740.58	Joback Method
cpg	588.64	J/mol×K	777.95	Joback Method
cpg	603.70	J/mol×K	815.33	Joback Method
cpg	617.63	J/mol×K	852.70	Joback Method
cpg	630.48	J/mol×K	890.08	Joback Method
dvisc	0.0017973	Pa×s	380.81	Joback Method
dvisc	0.0010085	Pa×s	428.31	Joback Method

dvisc	0.0006350	Pa×s	475.82	Joback Method
dvisc	0.0004349	Pa×s	523.32	Joback Method
dvisc	0.0003172	Pa×s	570.82	Joback Method
dvisc	0.0002429	Pa×s	618.33	Joback Method
dvisc	0.0001932	Pa×s	665.83	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307130&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
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

Latest version available from:
https://www.chemeo.com/cid/62-021-9/3-Cyclopentylpropionic-acid-3-methylphenyl-ester.pdf
Generated by Cheméo on 2024-04-29 15:57:18.295528901 +0000 UTC m=+16695487.216106214.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.