

3-Cyclopentylpropionic acid, 4-methoxyphenyl ester

Inchi:	InChI=1S/C15H20O3/c1-17-13-7-9-14(10-8-13)18-15(16)11-6-12-4-2-3-5-12/h7-10,12H,2
InchiKey:	MZZLAUVXFFQDCE-UHFFFAOYSA-N
Formula:	C15H20O3
SMILES:	COc1ccc(OC(=O)CCC2CCCC2)cc1
Mol. weight [g/mol]:	248.32

Physical Properties

Property code	Value	Unit	Source
gf	-124.17	kJ/mol	Joback Method
hf	-444.41	kJ/mol	Joback Method
hfus	26.17	kJ/mol	Joback Method
hvap	63.75	kJ/mol	Joback Method
log10ws	-4.07		Crippen Method
logp	3.571		Crippen Method
mvol	200.900	ml/mol	McGowan Method
pc	2197.95	kPa	Joback Method
rinpol	1964.00		NIST Webbook
rinpol	1964.00		NIST Webbook
tb	688.25	K	Joback Method
tc	909.68	K	Joback Method
tf	403.04	K	Joback Method
vc	0.750	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	564.36	J/molxK	688.25	Joback Method
cpg	643.12	J/molxK	872.77	Joback Method
cpg	629.71	J/molxK	835.87	Joback Method
cpg	615.16	J/molxK	798.96	Joback Method
cpg	599.43	J/molxK	762.06	Joback Method
cpg	582.51	J/molxK	725.15	Joback Method
cpg	655.41	J/molxK	909.68	Joback Method
dvisc	0.0001521	Paxs	688.25	Joback Method

dvisc	0.0001909	Paxs	640.72	Joback Method
dvisc	0.0002484	Paxs	593.18	Joback Method
dvisc	0.0003385	Paxs	545.64	Joback Method
dvisc	0.0004892	Paxs	498.11	Joback Method
dvisc	0.0007642	Paxs	450.58	Joback Method
dvisc	0.0013264	Paxs	403.04	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307133&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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