3-Cyclopentylpropionic acid, 2-propylphenyl ester

Inchi: InChI=1S/C17H24O2/c1-2-7-15-10-5-6-11-16(15)19-17(18)13-12-14-8-3-4-9-14/h5-6,10-

InchiKey: CINQQQWJKMNWCB-UHFFFAOYSA-N

Formula: C17H24O2

SMILES: CCCc1ccccc1OC(=O)CCC1CCCC1

Mol. weight [g/mol]: 260.37

Physical Properties

Property code	Value	Unit	Source
gf	-2.33	kJ/mol	Joback Method
hf	-353.47	kJ/mol	Joback Method
hfus	30.16	kJ/mol	Joback Method
hvap	65.79	kJ/mol	Joback Method
log10ws	-5.17		Crippen Method
logp	4.515		Crippen Method
mcvol	223.210	ml/mol	McGowan Method
pc	1877.28	kPa	Joback Method
rinpol	1998.00		NIST Webbook
tb	711.59	K	Joback Method
tc	928.42	K	Joback Method
tf	403.35	K	Joback Method
vc	0.845	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	645.86	J/mol×K	711.59	Joback Method
cpg	664.98	J/mol×K	747.73	Joback Method
cpg	682.83	J/mol×K	783.87	Joback Method
cpg	699.45	J/mol×K	820.01	Joback Method
cpg	714.89	J/mol×K	856.14	Joback Method
cpg	729.21	J/mol×K	892.28	Joback Method
cpg	742.44	J/mol×K	928.42	Joback Method
dvisc	0.0016129	Pa×s	403.35	Joback Method
dvisc	0.0008777	Pa×s	454.72	Joback Method

dvisc	0.0005404	Pa×s	506.10	Joback Method
dvisc	0.0003638	Pa×s	557.47	Joback Method
dvisc	0.0002619	Pa×s	608.84	Joback Method
dvisc	0.0001984	Pa×s	660.22	Joback Method
dvisc	0.0001564	Pa×s	711.59	Joback Method

Sources

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=U354333&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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