1,2-Cyclohexanedicarboxylic acid, 4-methoxyphenyl pentyl ester

Inchi: InChI=1S/C20H28O5/c1-3-4-7-14-24-19(21)17-8-5-6-9-18(17)20(22)25-16-12-10-15(23-2

InchiKey: SVOHNHYLSCXYPS-UHFFFAOYSA-N

Formula: C20H28O5

SMILES: CCCCCOC(=O)C1CCCCC1C(=O)Oc1ccc(OC)cc1

Mol. weight [g/mol]: 348.43

Physical Properties

Property code	Value	Unit	Source
gf	-335.80	kJ/mol	Joback Method
hf	-818.91	kJ/mol	Joback Method
hfus	40.88	kJ/mol	Joback Method
hvap	83.89	kJ/mol	Joback Method
log10ws	-4.78		Crippen Method
logp	4.140		Crippen Method
mcvol	278.790	ml/mol	McGowan Method
pc	1508.15	kPa	Joback Method
rinpol	2605.00		NIST Webbook
rinpol	2605.00		NIST Webbook
tb	878.54	K	Joback Method
tc	1097.07	K	Joback Method
tf	523.79	K	Joback Method
vc	1.046	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	906.14	J/mol×K	878.54	Joback Method
cpg	972.49	J/mol×K	1060.65	Joback Method
cpg	962.43	J/mol×K	1024.23	Joback Method
cpg	950.77	J/mol×K	987.81	Joback Method
cpg	937.51	J/mol×K	951.38	Joback Method
cpg	922.63	J/mol×K	914.96	Joback Method
cpg	980.95	J/mol×K	1097.07	Joback Method
dvisc	0.0000554	Pa×s	878.54	Joback Method

dvisc	0.0000704	Pa×s	819.41	Joback Method
dvisc	0.0000927	Pa×s	760.29	Joback Method
dvisc	0.0001281	Pa×s	701.16	Joback Method
dvisc	0.0001877	Pa×s	642.04	Joback Method
dvisc	0.0002973	Pa×s	582.91	Joback Method
dvisc	0.0005225	Pa×s	523.79	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339669&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume