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

Inchi: InChI=1S/C25H38O5/c1-3-4-5-6-7-8-9-12-19-29-24(26)22-13-10-11-14-23(22)25(27)30-2

InchiKey: HIYZMQYLHANDJG-UHFFFAOYSA-N

Formula: C25H38O5

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

Mol. weight [g/mol]: 418.57

Physical Properties

Property code	Value	Unit	Source
gf	-293.70	kJ/mol	Joback Method
hf	-922.11	kJ/mol	Joback Method
hfus	53.83	kJ/mol	Joback Method
hvap	95.02	kJ/mol	Joback Method
log10ws	-6.88		Crippen Method
logp	6.091		Crippen Method
mcvol	349.240	ml/mol	McGowan Method
pc	1071.46	kPa	Joback Method
rinpol	3115.00		NIST Webbook
rinpol	3115.00		NIST Webbook
tb	992.94	K	Joback Method
tc	1217.16	K	Joback Method
tf	580.14	K	Joback Method
vc	1.325	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1209.69	J/mol×K	992.94	Joback Method
cpg	1269.27	J/mol×K	1179.79	Joback Method
cpg	1261.10	J/mol×K	1142.42	Joback Method
cpg	1251.09	J/mol×K	1105.05	Joback Method
cpg	1239.20	J/mol×K	1067.68	Joback Method
cpg	1225.41	J/mol×K	1030.31	Joback Method
cpg	1275.62	J/mol×K	1217.16	Joback Method
dvisc	0.0000270	Pa×s	992.94	Joback Method

dvisc	0.0000348	Pa×s	924.14	Joback Method
dvisc	0.0000467	Pa×s	855.34	Joback Method
dvisc	0.0000660	Pa×s	786.54	Joback Method
dvisc	0.0000996	Pa×s	717.74	Joback Method
dvisc	0.0001641	Pa×s	648.94	Joback Method
dvisc	0.0003045	Pa×s	580.14	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=U339675&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