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

Inchi: InChI=1S/C21H30O5/c1-3-4-5-8-15-25-20(22)18-9-6-7-10-19(18)21(23)26-17-13-11-16(2

InchiKey: WVKDJCQEQDGWPJ-UHFFFAOYSA-N

Formula: C21H30O5

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

Mol. weight [g/mol]: 362.46

Physical Properties

Property code	Value	Unit	Source
gf	-327.38	kJ/mol	Joback Method
hf	-839.55	kJ/mol	Joback Method
hfus	43.47	kJ/mol	Joback Method
hvap	86.12	kJ/mol	Joback Method
log10ws	-5.20		Crippen Method
logp	4.530		Crippen Method
mcvol	292.880	ml/mol	McGowan Method
pc	1401.69	kPa	Joback Method
rinpol	2701.00		NIST Webbook
rinpol	2701.00		NIST Webbook
tb	901.42	K	Joback Method
tc	1119.46	K	Joback Method
tf	535.06	K	Joback Method
vc	1.101	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	965.93	J/mol×K	901.42	Joback Method
cpg	982.29	J/mol×K	937.76	Joback Method
cpg	996.98	J/mol×K	974.10	Joback Method
cpg	1010.02	J/mol×K	1010.44	Joback Method
cpg	1021.42	J/mol×K	1046.78	Joback Method
cpg	1031.18	J/mol×K	1083.12	Joback Method
cpg	1039.33	J/mol×K	1119.46	Joback Method
dvisc	0.0004725	Pa×s	535.06	Joback Method

dvisc	0.0002658	Pa×s	596.12	Joback Method
dvisc	0.0001664	Pa×s	657.18	Joback Method
dvisc	0.0001128	Pa×s	718.24	Joback Method
dvisc	0.0000813	Pa×s	779.30	Joback Method
dvisc	0.0000614	Pa×s	840.36	Joback Method
dvisc	0.0000482	Pa×s	901.42	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339671&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

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