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

Inchi: InChI=1S/C23H34O5/c1-3-4-5-6-7-10-17-27-22(24)20-11-8-9-12-21(20)23(25)28-19-15-1

InchiKey: UXGIHDAUTYRYBD-UHFFFAOYSA-N

Formula: C23H34O5

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

Mol. weight [g/mol]: 390.51

Physical Properties

Property code	Value	Unit	Source
gf	-310.54	kJ/mol	Joback Method
hf	-880.83	kJ/mol	Joback Method
hfus	48.65	kJ/mol	Joback Method
hvap	90.57	kJ/mol	Joback Method
log10ws	-6.04		Crippen Method
logp	5.311		Crippen Method
mcvol	321.060	ml/mol	McGowan Method
pc	1219.99	kPa	Joback Method
rinpol	2894.00		NIST Webbook
rinpol	2894.00		NIST Webbook
tb	947.18	K	Joback Method
tc	1166.57	K	Joback Method
tf	557.60	K	Joback Method
vc	1.214	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1087.02	J/mol×K	947.18	Joback Method
cpg	1149.69	J/mol×K	1130.01	Joback Method
cpg	1140.63	J/mol×K	1093.44	Joback Method
cpg	1129.85	J/mol×K	1056.88	Joback Method
cpg	1117.34	J/mol×K	1020.31	Joback Method
cpg	1103.06	J/mol×K	983.75	Joback Method
cpg	1157.04	J/mol×K	1166.57	Joback Method
dvisc	0.0000362	Pa×s	947.18	Joback Method

dvisc	0.0000464	Pa×s	882.25	Joback Method
dvisc	0.0000619	Pa×s	817.32	Joback Method
dvisc	0.0000867	Pa×s	752.39	Joback Method
dvisc	0.0001295	Pa×s	687.46	Joback Method
dvisc	0.0002102	Pa×s	622.53	Joback Method
dvisc	0.0003819	Pa×s	557.60	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U339673&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