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

Inchi: InChI=1S/C24H36O5/c1-3-4-5-6-7-8-11-18-28-23(25)21-12-9-10-13-22(21)24(26)29-20-1

InchiKey: DPZOHMJPAVZHIJ-UHFFFAOYSA-N

Formula: C24H36O5

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

Mol. weight [g/mol]: 404.54

Physical Properties

Property code	Value	Unit	Source
gf	-302.12	kJ/mol	Joback Method
hf	-901.47	kJ/mol	Joback Method
hfus	51.24	kJ/mol	Joback Method
hvap	92.80	kJ/mol	Joback Method
log10ws	-6.46		Crippen Method
logp	5.701		Crippen Method
mcvol	335.150	ml/mol	McGowan Method
pc	1142.12	kPa	Joback Method
rinpol	3013.00		NIST Webbook
rinpol	3013.00		NIST Webbook
tb	970.06	K	Joback Method
tc	1191.40	K	Joback Method
tf	568.87	K	Joback Method
vc	1.270	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1148.19	J/mol×K	970.06	Joback Method
cpg	1209.38	J/mol×K	1154.51	Joback Method
cpg	1200.74	J/mol×K	1117.62	Joback Method
cpg	1190.32	J/mol×K	1080.73	Joback Method
cpg	1178.11	J/mol×K	1043.84	Joback Method
cpg	1164.07	J/mol×K	1006.95	Joback Method
cpg	1216.26	J/mol×K	1191.40	Joback Method
dvisc	0.0000313	Pa×s	970.06	Joback Method

dvisc	0.0000402	Pa×s	903.19	Joback Method
dvisc	0.0000538	Pa×s	836.33	Joback Method
dvisc	0.0000757	Pa×s	769.46	Joback Method
dvisc	0.0001137	Pa×s	702.60	Joback Method
dvisc	0.0001860	Pa×s	635.74	Joback Method
dvisc	0.0003416	Pa×s	568.87	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=U339674&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