1,2-Cyclohexanedicarboxylic acid, heptyl 3-methylphenyl ester

Inchi: InChI=1S/C22H32O4/c1-3-4-5-6-9-15-25-21(23)19-13-7-8-14-20(19)22(24)26-18-12-10-1

InchiKey: HZSSQPISMQKMBH-UHFFFAOYSA-N

Formula: C22H32O4

SMILES: CCCCCCCOC(=O)C1CCCCC1C(=O)Oc1cccc(C)c1

Mol. weight [g/mol]: 360.49

Physical Properties

Property code	Value	Unit	Source
gf	-213.96	kJ/mol	Joback Method
hf	-727.97	kJ/mol	Joback Method
hfus	44.87	kJ/mol	Joback Method
hvap	85.94	kJ/mol	Joback Method
log10ws	-5.98		Crippen Method
logp	5.220		Crippen Method
mcvol	301.100	ml/mol	McGowan Method
pc	1322.31	kPa	Joback Method
rinpol	2623.00		NIST Webbook
rinpol	2623.00		NIST Webbook
tb	901.88	K	Joback Method
tc	1119.41	K	Joback Method
tf	524.10	K	Joback Method
vc	1.139	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	996.81	J/mol×K	901.88	Joback Method
cpg	1013.95	J/mol×K	938.13	Joback Method
cpg	1029.50	J/mol×K	974.39	Joback Method
cpg	1043.48	J/mol×K	1010.64	Joback Method
cpg	1055.92	J/mol×K	1046.90	Joback Method
cpg	1066.85	J/mol×K	1083.15	Joback Method
cpg	1076.30	J/mol×K	1119.41	Joback Method
dvisc	0.0006041	Pa×s	524.10	Joback Method

dvisc	0.0003285	Pa×s	587.06	Joback Method
dvisc	0.0002010	Pa×s	650.03	Joback Method
dvisc	0.0001341	Pa×s	712.99	Joback Method
dvisc	0.0000956	Pa×s	775.95	Joback Method
dvisc	0.0000717	Pa×s	838.92	Joback Method
dvisc	0.0000559	Pa×s	901.88	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=U339834&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