1,2-Cyclohexanedicarboxylic acid, 2,5-dimethylphenyl isohexyl ester

Inchi: InChI=1S/C22H32O4/c1-15(2)8-7-13-25-21(23)18-9-5-6-10-19(18)22(24)26-20-14-16(3)1

InchiKey: OYCANJDQPOAVHK-UHFFFAOYSA-N

Formula: C22H32O4

SMILES: Cc1ccc(C)c(OC(=O)C2CCCCC2C(=O)OCCCC(C)C)c1

Mol. weight [g/mol]: 360.49

Physical Properties

Property code	Value	Unit	Source
gf	-226.03	kJ/mol	Joback Method
hf	-744.72	kJ/mol	Joback Method
hfus	40.96	kJ/mol	Joback Method
hvap	86.21	kJ/mol	Joback Method
log10ws	-5.79		Crippen Method
logp	4.995		Crippen Method
mcvol	301.100	ml/mol	McGowan Method
pc	1315.61	kPa	Joback Method
rinpol	2541.00		NIST Webbook
rinpol	2541.00		NIST Webbook
tb	906.42	K	Joback Method
tc	1126.86	K	Joback Method
tf	521.62	K	Joback Method
vc	1.133	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	996.65	J/mol×K	906.42	Joback Method
cpg	1013.78	J/mol×K	943.16	Joback Method
cpg	1029.26	J/mol×K	979.90	Joback Method
cpg	1043.10	J/mol×K	1016.64	Joback Method
cpg	1055.33	J/mol×K	1053.38	Joback Method
cpg	1065.97	J/mol×K	1090.12	Joback Method
cpg	1075.05	J/mol×K	1126.86	Joback Method
dvisc	0.0005811	Pa×s	521.62	Joback Method

dvisc	0.0003119	Pa×s	585.75	Joback Method
dvisc	0.0001893	Pa×s	649.89	Joback Method
dvisc	0.0001257	Pa×s	714.02	Joback Method
dvisc	0.0000893	Pa×s	778.15	Joback Method
dvisc	0.0000668	Pa×s	842.29	Joback Method
dvisc	0.0000521	Pa×s	906.42	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=U339942&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