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

Inchi: InChI=1S/C24H36O4/c1-3-4-5-6-7-8-11-17-27-23(25)21-15-9-10-16-22(21)24(26)28-20-1

InchiKey: KIIJHWFOFLSFJI-UHFFFAOYSA-N

Formula: C24H36O4

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

Mol. weight [g/mol]: 388.54

Physical Properties

Property code	Value	Unit	Source
gf	-197.12	kJ/mol	Joback Method
hf	-769.25	kJ/mol	Joback Method
hfus	50.05	kJ/mol	Joback Method
hvap	90.39	kJ/mol	Joback Method
log10ws	-6.81		Crippen Method
logp	6.001		Crippen Method
mcvol	329.280	ml/mol	McGowan Method
pc	1155.35	kPa	Joback Method
rinpol	2826.00		NIST Webbook
rinpol	2826.00		NIST Webbook
tb	947.64	K	Joback Method
tc	1166.72	K	Joback Method
tf	546.64	K	Joback Method
vc	1.252	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1118.97	J/mol×K	947.64	Joback Method
cpg	1135.90	J/mol×K	984.15	Joback Method
cpg	1151.14	J/mol×K	1020.67	Joback Method
cpg	1164.74	J/mol×K	1057.18	Joback Method
cpg	1176.73	J/mol×K	1093.70	Joback Method
cpg	1187.14	J/mol×K	1130.21	Joback Method
cpg	1196.02	J/mol×K	1166.72	Joback Method
dvisc	0.0004883	Pa×s	546.64	Joback Method

dvisc	0.0002598	Pa×s	613.47	Joback Method
dvisc	0.0001565	Pa×s	680.31	Joback Method
dvisc	0.0001032	Pa×s	747.14	Joback Method
dvisc	0.0000729	Pa×s	813.97	Joback Method
dvisc	0.0000543	Pa×s	880.81	Joback Method
dvisc	0.0000421	Pa×s	947.64	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339836&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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