

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-
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	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0002598	Paxs	613.47	Joback Method
dvisc	0.0001565	Paxs	680.31	Joback Method
dvisc	0.0001032	Paxs	747.14	Joback Method
dvisc	0.0000729	Paxs	813.97	Joback Method
dvisc	0.0000543	Paxs	880.81	Joback Method
dvisc	0.0000421	Paxs	947.64	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339836&Units=SI

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

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