

1,2-Cyclohexanedicarboxylic acid, nonyl pentyl ester

Inchi:	InChI=1S/C22H40O4/c1-3-5-7-8-9-10-14-18-26-22(24)20-16-12-11-15-19(20)21(23)25-1
InchiKey:	BHGSZXWIVNXZEH-UHFFFAOYSA-N
Formula:	C22H40O4
SMILES:	CCCCCCCCCOC(=O)C1CCCCC1C(=O)OCCCCC
Mol. weight [g/mol]:	368.55

Physical Properties

Property code	Value	Unit	Source
gf	-316.74	kJ/mol	Joback Method
hf	-953.03	kJ/mol	Joback Method
hfus	51.22	kJ/mol	Joback Method
hvap	83.00	kJ/mol	Joback Method
log10ws	-6.17		Crippen Method
logp	5.820		Crippen Method
mvol	324.860	ml/mol	McGowan Method
pc	1063.79	kPa	Joback Method
rinpol	2529.00		NIST Webbook
rinpol	2529.00		NIST Webbook
tb	870.22	K	Joback Method
tc	1069.14	K	Joback Method
tf	485.16	K	Joback Method
vc	1.248	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1093.02	J/molxK	870.22	Joback Method
cpg	1176.19	J/molxK	1035.99	Joback Method
cpg	1162.35	J/molxK	1002.83	Joback Method
cpg	1147.13	J/molxK	969.68	Joback Method
cpg	1130.52	J/molxK	936.53	Joback Method
cpg	1112.49	J/molxK	903.37	Joback Method
cpg	1188.68	J/molxK	1069.14	Joback Method
dvisc	0.0000534	Paxs	870.22	Joback Method

dvisc	0.0000702	Paxs	806.04	Joback Method
dvisc	0.0000968	Paxs	741.87	Joback Method
dvisc	0.0001418	Paxs	677.69	Joback Method
dvisc	0.0002252	Paxs	613.51	Joback Method
dvisc	0.0003983	Paxs	549.34	Joback Method
dvisc	0.0008194	Paxs	485.16	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339472&Units=SI
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

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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