

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

Inchi:	InChI=1S/C22H40O4/c1-4-7-8-9-10-11-14-17-25-21(23)19-15-12-13-16-20(19)22(24)26-
InchiKey:	VZSJQINRZXYIGX-UHFFFAOYSA-N
Formula:	C22H40O4
SMILES:	CCCCCCCCCOC(=O)C1CCCCC1C(=O)OC(CC)CC
Mol. weight [g/mol]:	368.55

Physical Properties

Property code	Value	Unit	Source
gf	-319.18	kJ/mol	Joback Method
hf	-958.31	kJ/mol	Joback Method
hfus	47.69	kJ/mol	Joback Method
hvap	82.61	kJ/mol	Joback Method
log10ws	-6.28		Crippen Method
logp	5.818		Crippen Method
mvol	324.860	ml/mol	McGowan Method
pc	1069.36	kPa	Joback Method
rinpol	2441.00		NIST Webbook
rinpol	2441.00		NIST Webbook
tb	869.78	K	Joback Method
tc	1069.70	K	Joback Method
tf	470.16	K	Joback Method
vc	1.242	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1093.46	J/molxK	869.78	Joback Method
cpg	1176.80	J/molxK	1036.38	Joback Method
cpg	1162.98	J/molxK	1003.06	Joback Method
cpg	1147.76	J/molxK	969.74	Joback Method
cpg	1131.11	J/molxK	936.42	Joback Method
cpg	1113.02	J/molxK	903.10	Joback Method
cpg	1189.25	J/molxK	1069.70	Joback Method
dvisc	0.0000488	Paxs	869.78	Joback Method

dvisc	0.0000652	Paxs	803.18	Joback Method
dvisc	0.0000917	Paxs	736.57	Joback Method
dvisc	0.0001381	Paxs	669.97	Joback Method
dvisc	0.0002276	Paxs	603.37	Joback Method
dvisc	0.0004247	Paxs	536.76	Joback Method
dvisc	0.0009457	Paxs	470.16	Joback Method

Sources

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=U339507&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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