

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

Inchi:	InChI=1S/C26H40O4/c1-2-3-4-5-6-7-13-20-29-25(27)23-18-11-12-19-24(23)26(28)30-21
InchiKey:	KXABSGMJLXHOGX-UHFFFAOYSA-N
Formula:	C26H40O4
SMILES:	CCCCCCCCCOC(=O)C1CCCCC1C(=O)OCCc1ccccc1
Mol. weight [g/mol]:	416.59

Physical Properties

Property code	Value	Unit	Source
gf	-170.65	kJ/mol	Joback Method
hf	-799.06	kJ/mol	Joback Method
hfus	55.62	kJ/mol	Joback Method
hvap	94.18	kJ/mol	Joback Method
log10ws	-6.95		Crippen Method
logp	6.263		Crippen Method
mvol	357.460	ml/mol	McGowan Method
pc	1027.94	kPa	Joback Method
rinpol	3060.00		NIST Webbook
rinpol	3060.00		NIST Webbook
tb	988.42	K	Joback Method
tc	1211.55	K	Joback Method
tf	556.66	K	Joback Method
vc	1.363	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1243.48	J/molxK	988.42	Joback Method
cpg	1310.92	J/molxK	1174.36	Joback Method
cpg	1300.76	J/molxK	1137.17	Joback Method
cpg	1288.99	J/molxK	1099.98	Joback Method
cpg	1275.56	J/molxK	1062.80	Joback Method
cpg	1260.41	J/molxK	1025.61	Joback Method
cpg	1319.51	J/molxK	1211.55	Joback Method
dvisc	0.0000307	Paxs	988.42	Joback Method

dvisc	0.0000402	Paxs	916.46	Joback Method
dvisc	0.0000551	Paxs	844.50	Joback Method
dvisc	0.0000803	Paxs	772.54	Joback Method
dvisc	0.0001262	Paxs	700.58	Joback Method
dvisc	0.0002202	Paxs	628.62	Joback Method
dvisc	0.0004435	Paxs	556.66	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=U339500&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

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