

cis-Cyclohex-4-en-1,2-dicarboxylic acid, decyl nonyl ester

Inchi:	InChI=1S/C27H48O4/c1-3-5-7-9-11-13-15-19-23-31-27(29)25-21-17-16-20-24(25)26(28)
InchiKey:	HJSPLUVPOSVQPQ-UHFFFAOYSA-N
Formula:	C27H48O4
SMILES:	CCCCCCCCCOC(=O)C1CC=CCC1C(=O)OCCCCCCCCC
Mol. weight [g/mol]:	436.67

Physical Properties

Property code	Value	Unit	Source
gf	-244.68	kJ/mol	Joback Method
hf	-998.45	kJ/mol	Joback Method
hfus	65.39	kJ/mol	Joback Method
hvap	94.42	kJ/mol	Joback Method
log10ws	-8.11		Crippen Method
logp	7.546		Crippen Method
mvol	391.010	ml/mol	McGowan Method
pc	811.68	kPa	Joback Method
rinpol	2971.00		NIST Webbook
rinpol	2971.00		NIST Webbook
tb	983.78	K	Joback Method
tc	1206.49	K	Joback Method
tf	542.27	K	Joback Method
vc	1.514	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1378.93	J/molxK	983.78	Joback Method
cpg	1398.60	J/molxK	1020.90	Joback Method
cpg	1416.38	J/molxK	1058.02	Joback Method
cpg	1432.34	J/molxK	1095.13	Joback Method
cpg	1446.51	J/molxK	1132.25	Joback Method
cpg	1458.95	J/molxK	1169.37	Joback Method
cpg	1469.72	J/molxK	1206.49	Joback Method
dvisc	0.0004533	Paxs	542.27	Joback Method

dvisc	0.0002157	Paxs	615.86	Joback Method
dvisc	0.0001203	Paxs	689.44	Joback Method
dvisc	0.0000751	Paxs	763.03	Joback Method
dvisc	0.0000509	Paxs	836.61	Joback Method
dvisc	0.0000368	Paxs	910.20	Joback Method
dvisc	0.0000279	Paxs	983.78	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=U382678&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_cvol:	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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