

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

Inchi:	InChI=1S/C25H36O4/c1-2-3-4-5-6-7-13-19-28-24(26)22-16-11-12-17-23(22)25(27)29-20
InchiKey:	WQVWPIJEZPLOJW-UHFFFAOYSA-N
Formula:	C25H36O4
SMILES:	CCCCCCCCCOC(=O)C1CC=CCC1C(=O)OCCc1ccccc1
Mol. weight [g/mol]:	400.55

Physical Properties

Property code	Value	Unit	Source
gf	-149.11	kJ/mol	Joback Method
hf	-720.64	kJ/mol	Joback Method
hfus	54.25	kJ/mol	Joback Method
hvap	92.24	kJ/mol	Joback Method
log10ws	-6.38		Crippen Method
logp	5.649		Crippen Method
mvol	339.070	ml/mol	McGowan Method
pc	1120.80	kPa	Joback Method
rinpol	2910.00		NIST Webbook
rinpol	2910.00		NIST Webbook
tb	964.70	K	Joback Method
tc	1185.25	K	Joback Method
tf	546.15	K	Joback Method
vc	1.294	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1150.29	J/molxK	964.70	Joback Method
cpg	1166.67	J/molxK	1001.46	Joback Method
cpg	1181.39	J/molxK	1038.22	Joback Method
cpg	1194.51	J/molxK	1074.97	Joback Method
cpg	1206.08	J/molxK	1111.73	Joback Method
cpg	1216.15	J/molxK	1148.49	Joback Method
cpg	1224.78	J/molxK	1185.25	Joback Method
dvisc	0.0005009	Paxs	546.15	Joback Method

dvisc	0.0002572	Paxs	615.91	Joback Method
dvisc	0.0001512	Paxs	685.67	Joback Method
dvisc	0.0000981	Paxs	755.42	Joback Method
dvisc	0.0000684	Paxs	825.18	Joback Method
dvisc	0.0000505	Paxs	894.94	Joback Method
dvisc	0.0000389	Paxs	964.70	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382796&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

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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