

cis-Cyclohex-4-en-1,2-dicarboxylic acid, 3-methylbutyl tetradecyl ester

Inchi:	InChI=1S/C27H48O4/c1-4-5-6-7-8-9-10-11-12-13-14-17-21-30-26(28)24-18-15-16-19-25
InchiKey:	GDPNHIIFVXUVBX-UHFFFAOYSA-N
Formula:	C27H48O4
SMILES:	CCCCCCCCCCCCCOC(=O)C1CC=CCC1C(=O)OCCC(C)C
Mol. weight [g/mol]:	436.67

Physical Properties

Property code	Value	Unit	Source
gf	-247.12	kJ/mol	Joback Method
hf	-1003.73	kJ/mol	Joback Method
hfus	61.86	kJ/mol	Joback Method
hvap	94.03	kJ/mol	Joback Method
log10ws	-7.87		Crippen Method
logp	7.402		Crippen Method
mcvol	391.010	ml/mol	McGowan Method
pc	815.39	kPa	Joback Method
rinpol	2948.00		NIST Webbook
rinpol	2948.00		NIST Webbook
tb	983.34	K	Joback Method
tc	1205.22	K	Joback Method
tf	527.27	K	Joback Method
vc	1.508	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1379.25	J/molxK	983.34	Joback Method
cpg	1398.80	J/molxK	1020.32	Joback Method
cpg	1416.47	J/molxK	1057.30	Joback Method
cpg	1432.30	J/molxK	1094.28	Joback Method
cpg	1446.35	J/molxK	1131.26	Joback Method
cpg	1458.67	J/molxK	1168.24	Joback Method
cpg	1469.30	J/molxK	1205.22	Joback Method
dvisc	0.0005083	Paxs	527.27	Joback Method

dvisc	0.0002251	Paxs	603.28	Joback Method
dvisc	0.0001197	Paxs	679.29	Joback Method
dvisc	0.0000722	Paxs	755.31	Joback Method
dvisc	0.0000478	Paxs	831.32	Joback Method
dvisc	0.0000339	Paxs	907.33	Joback Method
dvisc	0.0000254	Paxs	983.34	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=U382831&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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