

cis-Cyclohex-4-en-1,2-dicarboxylic acid, dodecyl hexyl ester

Inchi:	InChI=1S/C26H46O4/c1-3-5-7-9-10-11-12-13-14-18-22-30-26(28)24-20-16-15-19-23(24)
InchiKey:	MLXBJYRUOLNLFX-UHFFFAOYSA-N
Formula:	C26H46O4
SMILES:	CCCCCCCCCCCCOC(=O)C1CC=CCC1C(=O)OCCCCC
Mol. weight [g/mol]:	422.64

Physical Properties

Property code	Value	Unit	Source
gf	-253.10	kJ/mol	Joback Method
hf	-977.81	kJ/mol	Joback Method
hfus	62.80	kJ/mol	Joback Method
hvap	92.19	kJ/mol	Joback Method
log10ws	-7.70		Crippen Method
logp	7.156		Crippen Method
mvol	376.920	ml/mol	McGowan Method
pc	857.97	kPa	Joback Method
rinpol	2876.00		NIST Webbook
rinpol	2876.00		NIST Webbook
tb	960.90	K	Joback Method
tc	1176.90	K	Joback Method
tf	531.00	K	Joback Method
vc	1.458	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1315.13	J/molxK	960.90	Joback Method
cpg	1395.22	J/molxK	1140.90	Joback Method
cpg	1382.54	J/molxK	1104.90	Joback Method
cpg	1368.23	J/molxK	1068.90	Joback Method
cpg	1352.26	J/molxK	1032.90	Joback Method
cpg	1334.58	J/molxK	996.90	Joback Method
cpg	1406.32	J/molxK	1176.90	Joback Method
dvisc	0.0000324	Paxs	960.90	Joback Method

dvisc	0.0000426	Paxs	889.25	Joback Method
dvisc	0.0000588	Paxs	817.60	Joback Method
dvisc	0.0000865	Paxs	745.95	Joback Method
dvisc	0.0001379	Paxs	674.30	Joback Method
dvisc	0.0002457	Paxs	602.65	Joback Method
dvisc	0.0005116	Paxs	531.00	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382669&Units=SI

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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