

cis-Cyclohex-4-en-1,2-dicarboxylic acid, propyl undecyl ester

Inchi:	InChI=1S/C22H38O4/c1-3-5-6-7-8-9-10-11-14-18-26-22(24)20-16-13-12-15-19(20)21(23)
InchiKey:	HCOHDZWUQKSKCY-UHFFFAOYSA-N
Formula:	C22H38O4
SMILES:	CCCCCCCCCOC(=O)C1CC=CCC1C(=O)OCCC
Mol. weight [g/mol]:	366.53

Physical Properties

Property code	Value	Unit	Source
gf	-286.78	kJ/mol	Joback Method
hf	-895.25	kJ/mol	Joback Method
hfus	52.44	kJ/mol	Joback Method
hvap	83.29	kJ/mol	Joback Method
log10ws	-6.02		Crippen Method
logp	5.596		Crippen Method
mcvol	320.560	ml/mol	McGowan Method
pc	1089.22	kPa	Joback Method
rinpol	2510.00		NIST Webbook
tb	869.38	K	Joback Method
tc	1068.63	K	Joback Method
tf	485.92	K	Joback Method
vc	1.234	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1063.97	J/molxK	869.38	Joback Method
cpg	1144.06	J/molxK	1035.42	Joback Method
cpg	1130.74	J/molxK	1002.21	Joback Method
cpg	1116.09	J/molxK	969.01	Joback Method
cpg	1100.10	J/molxK	935.80	Joback Method
cpg	1082.73	J/molxK	902.59	Joback Method
cpg	1156.08	J/molxK	1068.63	Joback Method
dvisc	0.0000578	Paxs	869.38	Joback Method
dvisc	0.0000753	Paxs	805.47	Joback Method

dvisc	0.0001027	Paxs	741.56	Joback Method
dvisc	0.0001484	Paxs	677.65	Joback Method
dvisc	0.0002318	Paxs	613.74	Joback Method
dvisc	0.0004013	Paxs	549.83	Joback Method
dvisc	0.0008030	Paxs	485.92	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=U382752&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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