

cis-Cyclohex-4-en-1,2-dicarboxylic acid, 2-methylpent-3-yl undecyl ester

Inchi:	InChI=1S/C25H44O4/c1-5-7-8-9-10-11-12-13-16-19-28-24(26)21-17-14-15-18-22(21)25(
InchiKey:	AFADIWIYBCMZSY-UHFFFAOYSA-N
Formula:	C25H44O4
SMILES:	CCCCCCCCCOC(=O)C1CC=CCC1C(=O)OC(CC)C(C)C
Mol. weight [g/mol]:	408.61

Physical Properties

Property code	Value	Unit	Source
gf	-266.40	kJ/mol	Joback Method
hf	-967.73	kJ/mol	Joback Method
hfus	53.16	kJ/mol	Joback Method
hvap	89.19	kJ/mol	Joback Method
log10ws	-7.15		Crippen Method
logp	6.621		Crippen Method
mvol	362.830	ml/mol	McGowan Method
pc	917.16	kPa	Joback Method
rinpol	2733.00		NIST Webbook
rinpol	2733.00		NIST Webbook
tb	937.14	K	Joback Method
tc	1147.64	K	Joback Method
tf	489.73	K	Joback Method
vc	1.389	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1252.47	J/molxK	937.14	Joback Method
cpg	1271.65	J/molxK	972.22	Joback Method
cpg	1289.16	J/molxK	1007.31	Joback Method
cpg	1305.04	J/molxK	1042.39	Joback Method
cpg	1319.32	J/molxK	1077.47	Joback Method
cpg	1332.04	J/molxK	1112.56	Joback Method
cpg	1343.25	J/molxK	1147.64	Joback Method
dvisc	0.0007476	Paxs	489.73	Joback Method

dvisc	0.0003104	Paxs	564.30	Joback Method
dvisc	0.0001582	Paxs	638.87	Joback Method
dvisc	0.0000929	Paxs	713.43	Joback Method
dvisc	0.0000603	Paxs	788.00	Joback Method
dvisc	0.0000422	Paxs	862.57	Joback Method
dvisc	0.0000312	Paxs	937.14	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=U382767&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
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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