

1,2-Cyclohexanedicarboxylic acid, dodecyl 2-isopropylphenyl ester

Inchi:	InChI=1S/C29H46O4/c1-4-5-6-7-8-9-10-11-12-17-22-32-28(30)25-19-13-14-20-26(25)29
InchiKey:	YFYCMVQWJDPEIK-UHFFFAOYSA-N
Formula:	C29H46O4
SMILES:	CCCCCCCCCCCCOC(=O)C1CCCCC1C(=O)Oc1cccc1C(C)C
Mol. weight [g/mol]:	458.67

Physical Properties

Property code	Value	Unit	Source
gf	-157.46	kJ/mol	Joback Method
hf	-877.73	kJ/mol	Joback Method
hfus	59.47	kJ/mol	Joback Method
hvap	101.13	kJ/mol	Joback Method
log10ws	-8.78		Crippen Method
logp	7.986		Crippen Method
mvol	399.730	ml/mol	McGowan Method
pc	857.97	kPa	Joback Method
rinpol	3216.00		NIST Webbook
rinpol	3216.00		NIST Webbook
tb	1061.60	K	Joback Method
tc	1300.30	K	Joback Method
tf	587.99	K	Joback Method
vc	1.526	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1431.03	J/molxK	1061.60	Joback Method
cpg	1447.49	J/molxK	1101.38	Joback Method
cpg	1461.84	J/molxK	1141.17	Joback Method
cpg	1474.15	J/molxK	1180.95	Joback Method
cpg	1484.49	J/molxK	1220.73	Joback Method
cpg	1492.93	J/molxK	1260.52	Joback Method
cpg	1499.54	J/molxK	1300.30	Joback Method
dvisc	0.0002946	Paxs	587.99	Joback Method

dvisc	0.0001406	Paxs	666.92	Joback Method
dvisc	0.0000785	Paxs	745.86	Joback Method
dvisc	0.0000490	Paxs	824.79	Joback Method
dvisc	0.0000332	Paxs	903.73	Joback Method
dvisc	0.0000239	Paxs	982.66	Joback Method
dvisc	0.0000181	Paxs	1061.60	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339706&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

Latest version available from:

<https://www.chemeo.com/cid/90-561-9/1-2-Cyclohexanedicarboxylic-acid-dodecyl-2-isopropylphenyl-ester.pdf>

Generated by Cheméo on 2026-05-17 17:32:36.796836547 +0000 UTC m=+2804505.854918768.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.