Isophthalic acid, 3,4-dimethylcyclohexyl pentyl ester

Inchi: InChI=1S/C21H30O4/c1-4-5-6-12-24-20(22)17-8-7-9-18(14-17)21(23)25-19-11-10-15(2)1

InchiKey: FIUZJZHTCWQPHA-UHFFFAOYSA-N

Formula: C21H30O4

SMILES: CCCCCOC(=O)c1cccc(C(=O)OC2CCC(C)C(C)C2)c1

Mol. weight [g/mol]: 346.46

Physical Properties

Property code	Value	Unit	Source
af	0.8671		Cheméo Relay (1.0)
hfus	46.51	kJ/mol	Joback Method
log10ws	-5.70		Cheméo Relay (1.0)
logp	5.015		Crippen Method
mcvol	287.010	ml/mol	McGowan Method
pc	1304.23	kPa	Joback Method
rinpol	2681.00		NIST Webbook
rinpol	2681.00		NIST Webbook
tb	653.46	K	Cheméo Relay (1.0)
tc	880.51	K	Cheméo Relay (1.0)
tf	288.89	K	Cheméo Relay (1.0)
vc	1.051	m3/kmol	Cheméo Relay (1.0)

Correlations

Information	Value
Property code	cpg
Equation	$Y = A + B \cdot T + C \cdot T^2 + D \cdot T^3 + E \cdot T.$
Y unit	J/mol×K
Coeff. A	-3.87160e+01
Coeff. B	1.81996e+00
Coeff. C	-8.63760e-04
Coeff. D	7.83000e-08
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00

Temperature range (K), max.	1000.00

Information	Value
Property code	dvisc
Equation	Y = exp(A + B/T + C·ln(T) + D·T^E)
Y unit	Pa×s
Coeff. A	-1.28642e+01
Coeff. B	2.67829e+03
Coeff. C	0.00000e+00
Coeff. D	0.00000e+00
Coeff. E	0.00000e+00
Basis	predicted
Comment	Liquid phase. Joback/Reid (1987), valid from Tf to 0.7·Tc.
Temperature range (K), min.	448.93
Temperature range (K), max.	736.27

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U343804&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

af: Acentric Factor

cpg: Ideal gas heat capacity

dvisc: Dynamic viscosity

hfus: Enthalpy of fusion 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/87-163-5/Isophthalic-acid-3-4-dimethylcyclohexyl-pentyl-ester.pdf
Generated by Cheméo on 2026-11-10 03:35:04.245988557 +0000 UTC m=+56815.174666780.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.