Isophthalic acid, pentadecyl 1-propylbutyl ester

Inchi: InChI=1S/C30H50O4/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-24-33-29(31)26-22-19-23-

InchiKey: IROXYTIINQUKNI-UHFFFAOYSA-N

Formula: C30H50O4

SMILES: CCCCCCCCCCCCCCCOC(=O)c1cccc(C(=O)OC(CCC)CCC)c1

Mol. weight [g/mol]: 474.73

Physical Properties

Property code	Value	Unit	Source
af	1.3236		Cheméo Relay (1.0)
hf	-1050.50	kJ/mol	Cheméo Relay (1.0)
hfus	72.32	kJ/mol	Joback Method
hvap	131.50	kJ/mol	Cheméo Relay (1.0)
log10ws	-8.46		Cheméo Relay (1.0)
logp	9.060		Crippen Method
mcvol	424.680	ml/mol	McGowan Method
pc	705.83	kPa	Joback Method
rinpol	3304.00		NIST Webbook
tb	699.93	K	Cheméo Relay (1.0)
tc	901.38	K	Cheméo Relay (1.0)
tf	277.69	K	Cheméo Relay (1.0)
vc	1.601	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	5.14800e+00
Coeff. B	2.61176e+00
Coeff. C	-1.38636e-03
Coeff. D	2.31700e-07
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	-1.55073e+01
Coeff. B	3.93466e+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.	536.46
Temperature range (K), max.	891.82

Sources

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):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U356410&Units=SI

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

Legend

af: Acentric Factor

cpg: Ideal gas heat capacity

dvisc: Dynamic viscosity

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/42-291-2/Isophthalic-acid-pentadecyl-1-propylbutyl-ester.pdf
Generated by Cheméo on 2026-11-07 22:54:48.841335377 +0000 UTC m=+18411.350572055.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.