

Phthalic acid, 3-iodobenzyl undecyl ester

Inchi:	InChI=1S/C26H33IO4/c1-2-3-4-5-6-7-8-9-12-18-30-25(28)23-16-10-11-17-24(23)26(29)3
InchiKey:	GHQCCDRHBZSQQB-UHFFFAOYSA-N
Formula:	C26H33IO4
SMILES:	CCCCCCCCCOC(=O)c1cccc1C(=O)OCc1cccc(I)c1
Mol. weight [g/mol]:	536.44

Physical Properties

Property code	Value	Unit	Source
gf	-36.12	kJ/mol	Joback Method
hf	-542.58	kJ/mol	Joback Method
hfus	60.38	kJ/mol	Joback Method
hvap	107.03	kJ/mol	Joback Method
log10ws	-9.40		Crippen Method
logp	7.336		Crippen Method
mcvol	370.380	ml/mol	McGowan Method
pc	1102.28	kPa	Joback Method
rinqol	3509.00		NIST Webbook
tb	1103.32	K	Joback Method
tc	1351.52	K	Joback Method
tf	663.04	K	Joback Method
vc	1.411	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1178.62	J/molxK	1103.32	Joback Method
cpg	1190.65	J/molxK	1144.69	Joback Method
cpg	1201.27	J/molxK	1186.05	Joback Method
cpg	1210.57	J/molxK	1227.42	Joback Method
cpg	1218.62	J/molxK	1268.79	Joback Method
cpg	1225.53	J/molxK	1310.16	Joback Method
cpg	1231.37	J/molxK	1351.52	Joback Method
dvisc	0.0001608	Paxs	663.04	Joback Method
dvisc	0.0000906	Paxs	736.42	Joback Method

dvisc	0.0000567	Paxs	809.80	Joback Method
dvisc	0.0000383	Paxs	883.18	Joback Method
dvisc	0.0000275	Paxs	956.56	Joback Method
dvisc	0.0000207	Paxs	1029.94	Joback Method
dvisc	0.0000162	Paxs	1103.32	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=U378075&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
mccvol:	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/23-165-3/Phthalic-acid-3-iodobenzyl-undecyl-ester.pdf>

Generated by Cheméo on 2024-05-02 20:25:02.961644518 +0000 UTC m=+16970751.882221834.

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