

Isophthalic acid, 2-propylphenyl tridecyl ester

Inchi:	InChI=1S/C30H42O4/c1-3-5-6-7-8-9-10-11-12-13-16-23-33-29(31)26-20-17-21-27(24-26
InchiKey:	XAEZBVGHKBDCLK-UHFFFAOYSA-N
Formula:	C30H42O4
SMILES:	CCCCCCCCCCCCOC(=O)c1cccc(C(=O)Oc2ccccc2CCC)c1
Mol. weight [g/mol]:	466.65

Physical Properties

Property code	Value	Unit	Source
gf	-60.56	kJ/mol	Joback Method
hf	-702.01	kJ/mol	Joback Method
hfus	66.33	kJ/mol	Joback Method
hvap	106.56	kJ/mol	Joback Method
log10ws	-10.05		Crippen Method
logp	8.326		Crippen Method
mvol	400.920	ml/mol	McGowan Method
pc	878.44	kPa	Joback Method
rinpol	3490.00		NIST Webbook
tb	1101.70	K	Joback Method
tc	1351.81	K	Joback Method
tf	650.06	K	Joback Method
vc	1.548	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1383.47	J/molxK	1101.70	Joback Method
cpg	1440.51	J/molxK	1310.12	Joback Method
cpg	1432.37	J/molxK	1268.44	Joback Method
cpg	1422.69	J/molxK	1226.75	Joback Method
cpg	1411.38	J/molxK	1185.07	Joback Method
cpg	1398.34	J/molxK	1143.38	Joback Method
cpg	1447.21	J/molxK	1351.81	Joback Method
dvisc	0.0000132	Paxs	1101.70	Joback Method
dvisc	0.0000170	Paxs	1026.43	Joback Method

dvisc	0.0000228	Paxs	951.15	Joback Method
dvisc	0.0000323	Paxs	875.88	Joback Method
dvisc	0.0000487	Paxs	800.61	Joback Method
dvisc	0.0000801	Paxs	725.33	Joback Method
dvisc	0.0001479	Paxs	650.06	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=U356635&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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