

Isophthalic acid, 4-tert-butylcyclohexyl undecyl ester

Inchi:	InChI=1S/C29H46O4/c1-5-6-7-8-9-10-11-12-13-21-32-27(30)23-15-14-16-24(22-23)28(3
InchiKey:	HVDFKDMIZOYSRE-UHFFFAOYSA-N
Formula:	C29H46O4
SMILES:	CCCCCCCCCOC(=O)c1cccc(C(=O)OC2CCC(C(C)(C)C)CC2)c1
Mol. weight [g/mol]:	458.67

Physical Properties

Property code	Value	Unit	Source
gf	-152.18	kJ/mol	Joback Method
hf	-881.20	kJ/mol	Joback Method
hfus	55.58	kJ/mol	Joback Method
hvap	100.22	kJ/mol	Joback Method
log10ws	-9.43		Crippen Method
logp	8.136		Crippen Method
mcvol	399.730	ml/mol	McGowan Method
pc	863.53	kPa	Joback Method
rinpol	3440.00		NIST Webbook
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tb	1058.81	K	Joback Method
tc	1296.32	K	Joback Method
tf	605.41	K	Joback Method
vc	1.520	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1430.90	J/molxK	1058.81	Joback Method
cpg	1447.79	J/molxK	1098.40	Joback Method
cpg	1462.80	J/molxK	1137.98	Joback Method
cpg	1476.04	J/molxK	1177.57	Joback Method
cpg	1487.58	J/molxK	1217.15	Joback Method
cpg	1497.55	J/molxK	1256.74	Joback Method
cpg	1506.02	J/molxK	1296.32	Joback Method
dvisc	0.0002306	Paxs	605.41	Joback Method

dvisc	0.0001133	Paxs	680.98	Joback Method
dvisc	0.0000642	Paxs	756.54	Joback Method
dvisc	0.0000403	Paxs	832.11	Joback Method
dvisc	0.0000273	Paxs	907.68	Joback Method
dvisc	0.0000197	Paxs	983.24	Joback Method
dvisc	0.0000149	Paxs	1058.81	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U345742&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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