Isophthalic acid, di(undec-2-en-1-yl) ester

Inchi: InChI=1S/C30H46O4/c1-3-5-7-9-11-13-15-17-19-24-33-29(31)27-22-21-23-28(26-27)30(
InchiKey: YHWOVSJMYXLLGW-XPWSMXQVSA-N
Formula: C30H46O4
SMILES: CCCCCCCCC=CCOC(=O)c1cccc(C(=O)OCC=CCCCCCCCC)c1
Mol. weight [g/mol]: 470.68

Physical Properties

Property code	Value	Unit	Source
gf	-2.90	kJ/mol	Joback Method
hf	-692.63	kJ/mol	Joback Method
hfus	73.09	kJ/mol	Joback Method
hvap	103.54	kJ/mol	Joback Method
log10ws	-10.04		Crippen Method
logp	8.614		Crippen Method
mcvol	416.080	ml/mol	McGowan Method
pc	777.64	kPa	Joback Method
rinpol	3483.00		NIST Webbook
rinpol	3483.00		NIST Webbook
tb	1078.36	K	Joback Method
tc	1328.34	K	Joback Method
tf	600.96	K	Joback Method
vc	1.615	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1439.49	J/mol×K	1078.36	Joback Method
cpg	1520.76	J/mol×K	1286.68	Joback Method
cpg	1506.93	J/mol×K	1245.02	Joback Method
cpg	1492.02	J/mol×K	1203.35	Joback Method
cpg	1475.90	J/mol×K	1161.69	Joback Method
cpg	1458.44	J/mol×K	1120.02	Joback Method
cpg	1533.65	J/mol×K	1328.34	Joback Method
dvisc	0.0000095	Pa×s	1078.36	Joback Method

dvisc	0.0000126	Pa×s	998.79	Joback Method
dvisc	0.0000175	Pa×s	919.23	Joback Method
dvisc	0.0000259	Pa×s	839.66	Joback Method
dvisc	0.0000417	Pa×s	760.09	Joback Method
dvisc	0.0000748	Pa×s	680.53	Joback Method
dvisc	0.0001569	Pa×s	600.96	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U343911&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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