

Isophthalic acid, cis-hex-3-enyl hexadecyl ester

Inchi:	InChI=1S/C30H48O4/c1-3-5-7-9-10-11-12-13-14-15-16-17-18-20-25-34-30(32)28-23-21-
InchiKey:	JEZFWWCBEPMPEJ-VURMDHGXSA-N
Formula:	C30H48O4
SMILES:	<chem>CCC=CCCOC(=O)c1cccc(C(=O)OCCCCCCCCCCCCCCC)c1</chem>
Mol. weight [g/mol]:	472.70

Physical Properties

Property code	Value	Unit	Source
gf	-83.12	kJ/mol	Joback Method
hf	-809.85	kJ/mol	Joback Method
hfus	72.88	kJ/mol	Joback Method
hvap	103.58	kJ/mol	Joback Method
log10ws	-10.18		Crippen Method
logp	8.838		Crippen Method
mcvol	420.380	ml/mol	McGowan Method
pc	755.57	kPa	Joback Method
rinpol	3452.00		NIST Webbook
tb	1074.20	K	Joback Method
tc	1326.23	K	Joback Method
tf	606.04	K	Joback Method
vc	1.635	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1468.16	J/molxK	1074.20	Joback Method
cpg	1487.11	J/molxK	1116.20	Joback Method
cpg	1504.29	J/molxK	1158.21	Joback Method
cpg	1519.79	J/molxK	1200.21	Joback Method
cpg	1533.75	J/molxK	1242.22	Joback Method
cpg	1546.28	J/molxK	1284.22	Joback Method
cpg	1557.50	J/molxK	1326.23	Joback Method
dvisc	0.0001694	Paxs	606.04	Joback Method
dvisc	0.0000824	Paxs	684.07	Joback Method

dvisc	0.0000464	Paxs	762.09	Joback Method
dvisc	0.0000291	Paxs	840.12	Joback Method
dvisc	0.0000198	Paxs	918.15	Joback Method
dvisc	0.0000143	Paxs	996.17	Joback Method
dvisc	0.0000108	Paxs	1074.20	Joback Method

Sources

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=U356710&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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