Isophthalic acid, di(2,6-dimethylnon-1-en-3-yn-5-yl) ester

Inchi: InChI=1S/C30H38O4/c1-9-12-23(7)27(18-16-21(3)4)33-29(31)25-14-11-15-26(20-25)30(

InchiKey: XVRBRLLOCVQTRB-UHFFFAOYSA-N

Formula: C30H38O4

SMILES: C=C(C)C#CC(OC(=O)c1cccc(C(=O)OC(C#CC(=C)C)C(C)CCC)c1)C(C)CCC

Mol. weight [g/mol]: 462.62

Physical Properties

Property code	Value	Unit	Source
gf	391.08	kJ/mol	Joback Method
hf	-172.31	kJ/mol	Joback Method
hfus	59.65	kJ/mol	Joback Method
hvap	105.20	kJ/mol	Joback Method
log10ws	-9.37		Crippen Method
logp	6.769		Crippen Method
mcvol	398.880	ml/mol	McGowan Method
pc	950.25	kPa	Joback Method
rinpol	3013.00		NIST Webbook
rinpol	3013.00		NIST Webbook
tb	1079.40	K	Joback Method
tc	1323.12	K	Joback Method
tf	731.88	K	Joback Method
vc	1.520	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1317.01	J/mol×K	1079.40	Joback Method
cpg	1331.98	J/mol×K	1120.02	Joback Method
cpg	1345.38	J/mol×K	1160.64	Joback Method
cpg	1357.30	J/mol×K	1201.26	Joback Method
cpg	1367.82	J/mol×K	1241.88	Joback Method
cpg	1377.03	J/mol×K	1282.50	Joback Method
cpg	1385.00	J/mol×K	1323.12	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U343857&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
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