Isophthalic acid, 3,7-dimethyloct-6-enyl dodecyl ester

Inchi: InChI=1S/C30H48O4/c1-5-6-7-8-9-10-11-12-13-14-22-33-29(31)27-19-16-20-28(24-27)3

InchiKey: URQMDQUUCUCMST-UHFFFAOYSA-N

Formula: C30H48O4

SMILES: CCCCCCCCCCCCOC(=O)c1cccc(C(=O)OCCC(C)CCC=C(C)C)c1

Mol. weight [g/mol]: 472.70

Physical Properties

Property code	Value	Unit	Source
gf	-94.11	kJ/mol	Joback Method
hf	-824.92	kJ/mol	Joback Method
hfus	68.05	kJ/mol	Joback Method
hvap	103.27	kJ/mol	Joback Method
log10ws	-9.94		Crippen Method
logp	8.694		Crippen Method
mcvol	420.380	ml/mol	McGowan Method
pc	761.00	kPa	Joback Method
rinpol	3384.00		NIST Webbook
tb	1073.64	K	Joback Method
tc	1322.23	K	Joback Method
tf	577.08	K	Joback Method
vc	1.631	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1468.06	J/mol×K	1073.64	Joback Method
cpg	1486.73	J/mol×K	1115.07	Joback Method
cpg	1503.66	J/mol×K	1156.50	Joback Method
cpg	1518.96	J/mol×K	1197.94	Joback Method
cpg	1532.74	J/mol×K	1239.37	Joback Method
cpg	1545.13	J/mol×K	1280.80	Joback Method
cpg	1556.22	J/mol×K	1322.23	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=U356745&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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