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

Inchi: InChI=1S/C29H46O4/c1-5-6-7-8-9-10-11-12-13-21-32-28(30)26-18-15-19-27(23-26)29(3

InchiKey: UQYBJKZUZFISSN-UHFFFAOYSA-N

Formula: C29H46O4

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

Mol. weight [g/mol]: 458.67

Physical Properties

Property code	Value	Unit	Source
gf	-102.53	kJ/mol	Joback Method
hf	-804.28	kJ/mol	Joback Method
hfus	65.46	kJ/mol	Joback Method
hvap	101.05	kJ/mol	Joback Method
log10ws	-9.52		Crippen Method
logp	8.304		Crippen Method
mcvol	406.290	ml/mol	McGowan Method
pc	802.97	kPa	Joback Method
rinpol	3285.00		NIST Webbook
tb	1050.76	K	Joback Method
tc	1290.45	K	Joback Method
tf	565.81	K	Joback Method
vc	1.575	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1404.30	J/mol×K	1050.76	Joback Method
cpg	1422.54	J/mol×K	1090.71	Joback Method
cpg	1439.14	J/mol×K	1130.66	Joback Method
cpg	1454.20	J/mol×K	1170.61	Joback Method
cpg	1467.83	J/mol×K	1210.56	Joback Method
cpg	1480.11	J/mol×K	1250.51	Joback Method
cpg	1491.16	J/mol×K	1290.45	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356744&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