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

Inchi: InChI=1S/C31H50O4/c1-5-6-7-8-9-10-11-12-13-14-15-23-34-30(32)28-20-17-21-29(25-2

InchiKey: LFXSFKAAERVRIU-UHFFFAOYSA-N

Formula: C31H50O4

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

Mol. weight [g/mol]: 486.73

Physical Properties

Property code	Value	Unit	Source
gf	-85.69	kJ/mol	Joback Method
hf	-845.56	kJ/mol	Joback Method
hfus	70.64	kJ/mol	Joback Method
hvap	105.50	kJ/mol	Joback Method
log10ws	-10.36		Crippen Method
logp	9.084		Crippen Method
mcvol	434.470	ml/mol	McGowan Method
pc	722.24	kPa	Joback Method
rinpol	3481.00		NIST Webbook
tb	1096.52	K	Joback Method
tc	1355.39	K	Joback Method
tf	588.35	K	Joback Method
vc	1.687	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1532.13	J/mol×K	1096.52	Joback Method
cpg	1551.30	J/mol×K	1139.66	Joback Method
cpg	1568.59	J/mol×K	1182.81	Joback Method
cpg	1584.16	J/mol×K	1225.95	Joback Method
cpg	1598.12	J/mol×K	1269.10	Joback Method
cpg	1610.63	J/mol×K	1312.24	Joback Method
cpg	1621.80	J/mol×K	1355.39	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356746&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
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