Isophthalic acid, trans-hex-3-enyl undecyl ester

Inchi: InChI=1S/C25H38O4/c1-3-5-7-9-10-11-12-13-15-20-29-25(27)23-18-16-17-22(21-23)24(

InchiKey: HFFLUYJIWSMQJV-SOFGYWHQSA-N

Formula: C25H38O4

SMILES: CCC=CCCOC(=O)c1cccc(C(=O)OCCCCCCCCCCC)c1

Mol. weight [g/mol]: 402.57

Physical Properties

Property code	Value	Unit	Source
gf	-125.22	kJ/mol	Joback Method
hf	-706.65	kJ/mol	Joback Method
hfus	59.93	kJ/mol	Joback Method
hvap	92.45	kJ/mol	Joback Method
log10ws	-8.09		Crippen Method
logp	6.887		Crippen Method
mcvol	349.930	ml/mol	McGowan Method
pc	1002.71	kPa	Joback Method
rinpol	2941.00		NIST Webbook
rinpol	2941.00		NIST Webbook
tb	959.80	K	Joback Method
tc	1175.26	K	Joback Method
tf	549.69	K	Joback Method
vc	1.355	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1153.14	J/mol×K	959.80	Joback Method
cpg	1170.06	J/mol×K	995.71	Joback Method
cpg	1185.67	J/mol×K	1031.62	Joback Method
cpg	1200.03	J/mol×K	1067.53	Joback Method
cpg	1213.20	J/mol×K	1103.44	Joback Method
cpg	1225.23	J/mol×K	1139.35	Joback Method
cpg	1236.18	J/mol×K	1175.26	Joback Method
dvisc	0.0003167	Pa×s	549.69	Joback Method

dvisc	0.0001611	Pa×s	618.04	Joback Method
dvisc	0.0000938	Pa×s	686.39	Joback Method
dvisc	0.0000602	Pa×s	754.74	Joback Method
dvisc	0.0000416	Pa×s	823.10	Joback Method
dvisc	0.0000304	Pa×s	891.45	Joback Method
dvisc	0.0000233	Pa×s	959.80	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=U356694&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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