

Isophthalic acid, hex-3-yl pentadecyl ester

Inchi:

InChI=1S/C29H48O4/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-23-32-28(30)25-21-19-22-

InchiKey:

LDVIHGREHMKNHI-UHFFFAOYSA-N

Formula:

C29H48O4

SMILES:

CCCCCCCCCCCCCCCCOC(=O)c1cccc(C(=O)OC(CC)CCC)c1

Mol. weight [g/mol]:

460.69

Physical Properties

Property code	Value	Unit	Source
gf	-174.20	kJ/mol	Joback Method
hf	-911.71	kJ/mol	Joback Method
hfus	66.57	kJ/mol	Joback Method
hvap	101.01	kJ/mol	Joback Method
log10ws	-10.02		Crippen Method
logp	8.670		Crippen Method
mcvol	410.590	ml/mol	McGowan Method
pc	777.64	kPa	Joback Method
rinpol	3349.00		NIST Webbook
rinpol	3349.00		NIST Webbook
tb	1046.72	K	Joback Method
tc	1288.88	K	Joback Method
tf	584.85	K	Joback Method
vc	1.593	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1433.30	J/mol×K	1046.72	Joback Method
cpg	1451.71	J/mol×K	1087.08	Joback Method
cpg	1468.21			

dvisc	0.0001073	Pa×s	661.83	Joback Method
dvisc	0.0000590	Pa×s	738.81	Joback Method
dvisc	0.0000363	Pa×s	815.78	Joback Method
dvisc	0.0000243	Pa×s	892.76	Joback Method
dvisc	0.0000173	Pa×s	969.74	Joback Method
dvisc	0.0000130	Pa×s	1046.72	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356480&Units=SI

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