Isophthalic acid, cis-hex-3-enyl pentadecyl ester

Inchi: InChI=1S/C29H46O4/c1-3-5-7-9-10-11-12-13-14-15-16-17-19-24-33-29(31)27-22-20-21-

InchiKey: YEISEMYWYSWCAK-VURMDHGXSA-N

Formula: C29H46O4

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

Mol. weight [g/mol]: 458.67

Physical Properties

Property code	Value	Unit	Source
gf	-91.54	kJ/mol	Joback Method
hf	-789.21	kJ/mol	Joback Method
hfus	70.29	kJ/mol	Joback Method
hvap	101.36	kJ/mol	Joback Method
log10ws	-9.76		Crippen Method
logp	8.448		Crippen Method
mcvol	406.290	ml/mol	McGowan Method
pc	797.08	kPa	Joback Method
rinpol	3351.00		NIST Webbook
tb	1051.32	K	Joback Method
tc	1293.56	K	Joback Method
tf	594.77	K	Joback Method
vc	1.579	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1404.37	J/mol×K	1051.32	Joback Method
cpg	1422.82	J/mol×K	1091.69	Joback Method
cpg	1439.62	J/mol×K	1132.07	Joback Method
cpg	1454.85	J/mol×K	1172.44	Joback Method
cpg	1468.62	J/mol×K	1212.81	Joback Method
cpg	1481.02	J/mol×K	1253.18	Joback Method
cpg	1492.17	J/mol×K	1293.56	Joback Method
dvisc	0.0001929	Pa×s	594.77	Joback Method
dvisc	0.0000946	Pa×s	670.86	Joback Method

dvisc	0.0000537	Pa×s	746.95	Joback Method
dvisc	0.0000338	Pa×s	823.04	Joback Method
dvisc	0.0000230	Pa×s	899.14	Joback Method
dvisc	0.0000166	Pa×s	975.23	Joback Method
dvisc	0.0000126	Pa×s	1051.32	Joback Method

Sources

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=U356709&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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