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

Inchi: InChI=1S/C26H40O4/c1-3-5-7-9-10-11-12-13-14-16-21-30-26(28)24-19-17-18-23(22-24)25(27)29-20-15-8-6-4-2/h3,5,15,17-19,22H,4,6-14,16,20-21H2,1-2H3/b5-3+,15-8+

InchiKey: KTVGKSFJJUMFRS-SOFGYWHQSA-N

Formula: C26H40O4

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

Mol. weight [g/mol]: 416.59

Physical Properties

Property code	Value	Unit	Source
gf	-116.80	kJ/mol	Joback Method
hf	-727.29	kJ/mol	Joback Method
hfus	62.52	kJ/mol	Joback Method
hvap	94.68	kJ/mol	Joback Method
log10ws	-8.51		Crippen Method
logp	7.277		Crippen Method
mcvol	364.020	ml/mol	McGowan Method
pc	944.42	kPa	Joback Method
rinpol	3043.00		NIST Webbook
rinpol	3043.00		NIST Webbook
tb	982.68	K	Joback Method
tc	1203.15	K	Joback Method
tf	560.96	K	Joback Method
vc	1.411	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1215.28	J/mol×K	982.68	Joback Method
cpg	1288.35	J/mol×K	1166.41	Joback Method
cpg	1276.23	J/mol×K	1129.66	Joback Method
cpg	1262.94	J/mol×K	1092.92	Joback Method
cpg	1248.39	J/mol×K	1056.17	Joback Method
cpg	1232.52	J/mol×K	1019.43	Joback Method
cpg	1299.34	J/mol×K	1203.15	Joback Method
dvisc	0.0000200	Pa×s	982.68	Joback Method

dvisc	0.0000262	Pa×s	912.39	Joback Method
dvisc	0.0000360	Pa×s	842.11	Joback Method
dvisc	0.0000523	Pa×s	771.82	Joback Method
dvisc	0.0000818	Pa×s	701.53	Joback Method
dvisc	0.0001416	Pa×s	631.25	Joback Method
dvisc	0.0002809	Pa×s	560.96	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=U356695&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