Isophthalic acid, dodecyl hex-3-yl ester

Inchi: InChI=1S/C26H42O4/c1-4-7-8-9-10-11-12-13-14-15-20-29-25(27)22-18-16-19-23(21-22)26(28)30-24(5-2)6-3/h16,18-19,21,24H,4-15,17,20H2,1-3H3

InchiKey: KCCHKWHKEYQJAF-UHFFFAOYSA-N

Formula: C26H42O4

SMILES: CCCCCCCCCCCCOC(=O)c1cccc(C(=O)OC(CC)CCC)c1

Mol. weight [g/mol]: 418.61

Physical Properties

Property code	Value	Unit	Source
gf	-199.46	kJ/mol	Joback Method
hf	-849.79	kJ/mol	Joback Method
hfus	58.80	kJ/mol	Joback Method
hvap	94.33	kJ/mol	Joback Method
log10ws	-8.77		Crippen Method
logp	7.500		Crippen Method
mcvol	368.320	ml/mol	McGowan Method
pc	919.39	kPa	Joback Method
rinpol	3038.00		NIST Webbook
tb	978.08	K	Joback Method
tc	1197.65	K	Joback Method
tf	551.04	K	Joback Method
vc	1.425	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1244.04	J/mol×K	978.08	Joback Method
cpg	1316.49	J/mol×K	1161.05	Joback Method
cpg	1304.90	J/mol×K	1124.46	Joback Method
cpg	1291.91	J/mol×K	1087.86	Joback Method
cpg	1277.47	J/mol×K	1051.27	Joback Method
cpg	1261.53	J/mol×K	1014.67	Joback Method
cpg	1326.73	J/mol×K	1197.65	Joback Method
dvisc	0.0000207	Pa×s	978.08	Joback Method
dvisc	0.0000275	Pa×s	906.91	Joback Method

dvisc	0.0000383	Pa×s	835.73	Joback Method
dvisc	0.0000566	Pa×s	764.56	Joback Method
dvisc	0.0000907	Pa×s	693.39	Joback Method
dvisc	0.0001620	Pa×s	622.21	Joback Method
dvisc	0.0003362	Pa×s	551.04	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=U356483&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