Isophthalic acid, dodecyl phenylethyl ester

Inchi: InChI=1S/C28H38O4/c1-2-3-4-5-6-7-8-9-10-14-21-31-27(29)25-18-15-19-26(23-25)28(30
InchiKey: ALYNKZJDNNWBSM-UHFFFAOYSA-N
Formula: C28H38O4
SMILES: CCCCCCCCCCCCOC(=O)c1cccc(C(=O)OCCc2ccccc2)c1
Mol. weight [g/mol]: 438.60

Physical Properties

Property code	Value	Unit	Source
gf	-67.77	kJ/mol	Joback Method
hf	-649.26	kJ/mol	Joback Method
hfus	61.54	kJ/mol	Joback Method
hvap	101.45	kJ/mol	Joback Method
log10ws	-8.59		Crippen Method
logp	7.164		Crippen Method
mcvol	372.740	ml/mol	McGowan Method
pc	997.02	kPa	Joback Method
rinpol	3521.00		NIST Webbook
rinpol	3521.00		NIST Webbook
tb	1050.96	K	Joback Method
tc	1286.69	K	Joback Method
tf	615.00	K	Joback Method
vc	1.435	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1260.53	J/mol×K	1050.96	Joback Method
cpg	1319.51	J/mol×K	1247.40	Joback Method
cpg	1310.57	J/mol×K	1208.11	Joback Method
cpg	1300.28	J/mol×K	1168.83	Joback Method
cpg	1288.56	J/mol×K	1129.54	Joback Method
cpg	1275.34	J/mol×K	1090.25	Joback Method
cpg	1327.18	J/mol×K	1286.69	Joback Method
dvisc	0.0000174	Pa×s	1050.96	Joback Method

dvisc	0.0000226	Pa×s	978.30	Joback Method
dvisc	0.0000306	Pa×s	905.64	Joback Method
dvisc	0.0000437	Pa×s	832.98	Joback Method
dvisc	0.0000668	Pa×s	760.32	Joback Method
dvisc	0.0001118	Pa×s	687.66	Joback Method
dvisc	0.0002110	Pa×s	615.00	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=U344342&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