Isophthalic acid, 2-isopropylphenyl undecyl ester

Inchi: InChI=1S/C28H38O4/c1-4-5-6-7-8-9-10-11-14-20-31-27(29)23-16-15-17-24(21-23)28(30)
InchiKey: OQDGMYUEKMWMQO-UHFFFAOYSA-N
Formula: C28H38O4
SMILES: CCCCCCCCCCCOC(=O)c1cccc(C(=O)Oc2ccccc2C(C)C)c1
Mol. weight [g/mol]: 438.60

Physical Properties

Property code	Value	Unit	Source
gf	-79.84	kJ/mol	Joback Method
hf	-666.01	kJ/mol	Joback Method
hfus	57.63	kJ/mol	Joback Method
hvap	101.72	kJ/mol	Joback Method
log10ws	-9.17		Crippen Method
logp	7.717		Crippen Method
mcvol	372.740	ml/mol	McGowan Method
pc	992.63	kPa	Joback Method
rinpol	3346.00		NIST Webbook
rinpol	3346.00		NIST Webbook
tb	1055.50	K	Joback Method
tc	1292.24	K	Joback Method
tf	612.52	K	Joback Method
vc	1.429	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1259.67	J/mol×K	1055.50	Joback Method
cpg	1274.17	J/mol×K	1094.96	Joback Method
cpg	1287.03	J/mol×K	1134.41	Joback Method
cpg	1298.31	J/mol×K	1173.87	Joback Method
cpg	1308.07	J/mol×K	1213.32	Joback Method
cpg	1316.40	J/mol×K	1252.78	Joback Method
cpg	1323.36	J/mol×K	1292.24	Joback Method
dvisc	0.0002032	Pa×s	612.52	Joback Method

dvisc	0.0001064	Pa×s	686.35	Joback Method
dvisc	0.0000631	Pa×s	760.18	Joback Method
dvisc	0.0000411	Pa×s	834.01	Joback Method
dvisc	0.0000287	Pa×s	907.84	Joback Method
dvisc	0.0000211	Pa×s	981.67	Joback Method
dvisc	0.0000163	Pa×s	1055.50	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=U344640&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