Isophthalic acid, 2-propylphenyl undecyl ester

Inchi: InChI=1S/C28H38O4/c1-3-5-6-7-8-9-10-11-14-21-31-27(29)24-18-15-19-25(22-24)28(30
InchiKey: XWSOSMMNIULZQM-UHFFFAOYSA-N
Formula: C28H38O4
SMILES: CCCCCCCCCCCOC(=O)c1cccc(C(=O)Oc2ccccc2CCC)c1
Mol. weight [g/mol]: 438.60

Physical Properties

Property code	Value	Unit	Source
gf	-77.40	kJ/mol	Joback Method
hf	-660.73	kJ/mol	Joback Method
hfus	61.15	kJ/mol	Joback Method
hvap	102.11	kJ/mol	Joback Method
log10ws	-9.21		Crippen Method
logp	7.546		Crippen Method
mcvol	372.740	ml/mol	McGowan Method
pc	987.64	kPa	Joback Method
rinpol	3284.00		NIST Webbook
rinpol	3284.00		NIST Webbook
tb	1055.94	K	Joback Method
tc	1292.80	K	Joback Method
tf	627.52	K	Joback Method
vc	1.435	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1259.42	J/mol×K	1055.94	Joback Method
cpg	1316.78	J/mol×K	1253.33	Joback Method
cpg	1308.30	J/mol×K	1213.85	Joback Method
cpg	1298.39	J/mol×K	1174.37	Joback Method
cpg	1286.99	J/mol×K	1134.89	Joback Method
cpg	1274.03	J/mol×K	1095.42	Joback Method
cpg	1323.91	J/mol×K	1292.80	Joback Method
dvisc	0.0000179	Pa×s	1055.94	Joback Method

dvisc	0.0000230	Pa×s	984.54	Joback Method
dvisc	0.0000308	Pa×s	913.13	Joback Method
dvisc	0.0000432	Pa×s	841.73	Joback Method
dvisc	0.0000645	Pa×s	770.33	Joback Method
dvisc	0.0001046	Pa×s	698.92	Joback Method
dvisc	0.0001895	Pa×s	627.52	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356633&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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