Phthalic acid, di(2-propylphenyl) ester

Inchi: InChI=1S/C26H26O4/c1-3-11-19-13-5-9-17-23(19)29-25(27)21-15-7-8-16-22(21)26(28)3
InchiKey: DPXRFHZIYSAEEK-UHFFFAOYSA-N
Formula: C26H26O4
SMILES: CCCc1ccccc1OC(=O)c1ccccc1C(=O)Oc1ccccc1CCC
Mol. weight [g/mol]: 402.48

Physical Properties

Property code	Value	Unit	Source
gf	8.54	kJ/mol	Joback Method
hf	-394.39	kJ/mol	Joback Method
hfus	49.63	kJ/mol	Joback Method
hvap	100.60	kJ/mol	Joback Method
log10ws	-8.09		Crippen Method
logp	6.030		Crippen Method
mcvol	320.800	ml/mol	McGowan Method
pc	1398.55	kPa	Joback Method
rinpol	2961.00		NIST Webbook
rinpol	2961.00		NIST Webbook
tb	1041.84	K	Joback Method
tc	1286.86	K	Joback Method
tf	643.92	K	Joback Method
vc	1.216	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1024.63	J/mol×K	1041.84	Joback Method
cpg	1036.26	J/mol×K	1082.68	Joback Method
cpg	1046.34	J/mol×K	1123.51	Joback Method
cpg	1054.95	J/mol×K	1164.35	Joback Method
cpg	1062.15	J/mol×K	1205.19	Joback Method
cpg	1068.01	J/mol×K	1246.02	Joback Method
cpg	1072.61	J/mol×K	1286.86	Joback Method
dvisc	0.0001999	Pa×s	643.92	Joback Method

dvisc	0.0001214	Pa×s	710.24	Joback Method
dvisc	0.0000802	Pa×s	776.56	Joback Method
dvisc	0.0000566	Pa×s	842.88	Joback Method
dvisc	0.0000420	Pa×s	909.20	Joback Method
dvisc	0.0000325	Pa×s	975.52	Joback Method
dvisc	0.0000260	Pa×s	1041.84	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357031&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

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

Latest version available from:
https://www.chemeo.com/cid/39-987-4/Phthalic-acid-di-2-propylphenyl-ester.pdf
Generated by Cheméo on 2024-10-12 03:10:54.715389145 +0000 UTC m=+3283517.352358404.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.