Phthalic acid, decyl 2-propylphenyl ester

Inchi: InChI=1S/C27H36O4/c1-3-5-6-7-8-9-10-15-21-30-26(28)23-18-12-13-19-24(23)27(29)31
InchiKey: RXKUUEJNPQUJGH-UHFFFAOYSA-N
Formula: C27H36O4
SMILES: CCCCCCCCCCOC(=O)c1ccccc1C(=O)Oc1ccccc1CCC
Mol. weight [g/mol]: 424.57

Physical Properties

Property code	Value	Unit	Source
gf	-85.82	kJ/mol	Joback Method
hf	-640.09	kJ/mol	Joback Method
hfus	58.56	kJ/mol	Joback Method
hvap	99.88	kJ/mol	Joback Method
log10ws	-8.79		Crippen Method
logp	7.156		Crippen Method
mcvol	358.650	ml/mol	McGowan Method
pc	1050.05	kPa	Joback Method
rinpol	3032.00		NIST Webbook
rinpol	3032.00		NIST Webbook
tb	1033.06	K	Joback Method
tc	1265.06	K	Joback Method
tf	616.25	K	Joback Method
vc	1.379	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1197.89	J/mol×K	1033.06	Joback Method
cpg	1212.40	J/mol×K	1071.73	Joback Method
cpg	1225.34	J/mol×K	1110.39	Joback Method
cpg	1236.78	J/mol×K	1149.06	Joback Method
cpg	1246.78	J/mol×K	1187.73	Joback Method
cpg	1255.41	J/mol×K	1226.39	Joback Method
cpg	1262.73	J/mol×K	1265.06	Joback Method
dvisc	0.0002136	Pa×s	616.25	Joback Method

dvisc	0.0001191	Pa×s	685.72	Joback Method
dvisc	0.0000739	Pa×s	755.19	Joback Method
dvisc	0.0000497	Pa×s	824.65	Joback Method
dvisc	0.0000356	Pa×s	894.12	Joback Method
dvisc	0.0000267	Pa×s	963.59	Joback Method
dvisc	0.0000209	Pa×s	1033.06	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=U357025&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

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