

Phthalic acid, dodecyl 2-propylphenyl ester

Inchi:	InChI=1S/C29H40O4/c1-3-5-6-7-8-9-10-11-12-17-23-32-28(30)25-20-14-15-21-26(25)29
InchiKey:	QNUVPCXQCRBRRP-UHFFFAOYSA-N
Formula:	C29H40O4
SMILES:	CCCCCCCCCCCCOC(=O)c1ccccc1C(=O)Oc1ccccc1CCC
Mol. weight [g/mol]:	452.63

Physical Properties

Property code	Value	Unit	Source
gf	-68.98	kJ/mol	Joback Method
hf	-681.37	kJ/mol	Joback Method
hfus	63.74	kJ/mol	Joback Method
hvap	104.34	kJ/mol	Joback Method
log10ws	-9.63		Crippen Method
logp	7.936		Crippen Method
mcvol	386.830	ml/mol	McGowan Method
pc	930.64	kPa	Joback Method
rinpol	3236.00		NIST Webbook
tb	1078.82	K	Joback Method
tc	1321.69	K	Joback Method
tf	638.79	K	Joback Method
vc	1.492	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1321.30	J/molxK	1078.82	Joback Method
cpg	1336.02	J/molxK	1119.30	Joback Method
cpg	1349.02	J/molxK	1159.78	Joback Method
cpg	1360.37	J/molxK	1200.26	Joback Method
cpg	1370.17	J/molxK	1240.74	Joback Method
cpg	1378.49	J/molxK	1281.22	Joback Method
cpg	1385.41	J/molxK	1321.69	Joback Method
dvisc	0.0001676	Paxs	638.79	Joback Method
dvisc	0.0000917	Paxs	712.13	Joback Method

dvisc	0.0000561	Paxs	785.47	Joback Method
dvisc	0.0000374	Paxs	858.81	Joback Method
dvisc	0.0000265	Paxs	932.14	Joback Method
dvisc	0.0000198	Paxs	1005.48	Joback Method
dvisc	0.0000154	Paxs	1078.82	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U357027&Units=SI

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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