

Dodecanoic acid, 2-propylphenyl ester

Inchi:	InChI=1S/C21H34O2/c1-3-5-6-7-8-9-10-11-12-18-21(22)23-20-17-14-13-16-19(20)15-4-2
InchiKey:	SUJMEWJAWIXHRY-UHFFFAOYSA-N
Formula:	C21H34O2
SMILES:	CCCCCCCCCCCC(=O)Oc1ccccc1CCC
Mol. weight [g/mol]:	318.49

Physical Properties

Property code	Value	Unit	Source
gf	-5.20	kJ/mol	Joback Method
hf	-496.51	kJ/mol	Joback Method
hfus	46.58	kJ/mol	Joback Method
hvap	74.43	kJ/mol	Joback Method
log10ws	-7.19		Crippen Method
logp	6.465		Crippen Method
mvol	290.430	ml/mol	McGowan Method
pc	1212.36	kPa	Joback Method
rinpol	2321.00		NIST Webbook
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tb	787.83	K	Joback Method
tc	979.38	K	Joback Method
tf	437.53	K	Joback Method
vc	1.127	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	885.17	J/molxK	787.83	Joback Method
cpg	967.02	J/molxK	947.45	Joback Method
cpg	952.64	J/molxK	915.53	Joback Method
cpg	937.30	J/molxK	883.60	Joback Method
cpg	920.96	J/molxK	851.68	Joback Method
cpg	903.60	J/molxK	819.75	Joback Method
cpg	980.48	J/molxK	979.38	Joback Method
dvisc	0.0000654	Paxs	787.83	Joback Method

dvisc	0.0000854	Paxs	729.45	Joback Method
dvisc	0.0001170	Paxs	671.06	Joback Method
dvisc	0.0001702	Paxs	612.68	Joback Method
dvisc	0.0002679	Paxs	554.30	Joback Method
dvisc	0.0004692	Paxs	495.91	Joback Method
dvisc	0.0009543	Paxs	437.53	Joback Method

Sources

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=U360545&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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