

5-Phenylvaleric acid, decyl ester

Inchi:	InChI=1S/C21H34O2/c1-2-3-4-5-6-7-8-14-19-23-21(22)18-13-12-17-20-15-10-9-11-16-20
InchiKey:	YBLXZQYXKMJFIF-UHFFFAOYSA-N
Formula:	C21H34O2
SMILES:	CCCCCCCCCOC(=O)CCCCc1ccccc1
Mol. weight [g/mol]:	318.49

Physical Properties

Property code	Value	Unit	Source
gf	4.43	kJ/mol	Joback Method
hf	-485.04	kJ/mol	Joback Method
hfus	46.97	kJ/mol	Joback Method
hvap	73.77	kJ/mol	Joback Method
log10ws	-6.58		Crippen Method
logp	6.083		Crippen Method
mvol	290.430	ml/mol	McGowan Method
pc	1225.12	kPa	Joback Method
rinpol	2402.00		NIST Webbook
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tb	782.85	K	Joback Method
tc	973.54	K	Joback Method
tf	425.01	K	Joback Method
vc	1.127	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	885.32	J/molxK	782.85	Joback Method
cpg	903.84	J/molxK	814.63	Joback Method
cpg	921.29	J/molxK	846.41	Joback Method
cpg	937.70	J/molxK	878.19	Joback Method
cpg	953.12	J/molxK	909.98	Joback Method
cpg	967.58	J/molxK	941.76	Joback Method
cpg	981.13	J/molxK	973.54	Joback Method
dvisc	0.0011705	Paxs	425.01	Joback Method

dvisc	0.0005373	Paxs	484.65	Joback Method
dvisc	0.0002925	Paxs	544.29	Joback Method
dvisc	0.0001796	Paxs	603.93	Joback Method
dvisc	0.0001203	Paxs	663.57	Joback Method
dvisc	0.0000861	Paxs	723.21	Joback Method
dvisc	0.0000649	Paxs	782.85	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=U406079&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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