

5-Phenylvaleric acid, undecyl ester

Inchi:	InChI=1S/C22H36O2/c1-2-3-4-5-6-7-8-9-15-20-24-22(23)19-14-13-18-21-16-11-10-12-17
InchiKey:	DLQQNBPDQMMYKD-UHFFFAOYSA-N
Formula:	C22H36O2
SMILES:	CCCCCCCCCOC(=O)CCCCc1ccccc1
Mol. weight [g/mol]:	332.52

Physical Properties

Property code	Value	Unit	Source
gf	12.85	kJ/mol	Joback Method
hf	-505.68	kJ/mol	Joback Method
hfus	49.56	kJ/mol	Joback Method
hvap	76.00	kJ/mol	Joback Method
log10ws	-7.00		Crippen Method
logp	6.473		Crippen Method
mvol	304.520	ml/mol	McGowan Method
pc	1146.76	kPa	Joback Method
rinpol	2509.00		NIST Webbook
rinpol	2509.00		NIST Webbook
tb	805.73	K	Joback Method
tc	997.16	K	Joback Method
tf	436.28	K	Joback Method
vc	1.183	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	945.31	J/molxK	805.73	Joback Method
cpg	964.06	J/molxK	837.63	Joback Method
cpg	981.72	J/molxK	869.54	Joback Method
cpg	998.31	J/molxK	901.44	Joback Method
cpg	1013.89	J/molxK	933.35	Joback Method
cpg	1028.49	J/molxK	965.25	Joback Method
cpg	1042.15	J/molxK	997.16	Joback Method
dvisc	0.0010554	Paxs	436.28	Joback Method

dvisc	0.0004794	Paxs	497.85	Joback Method
dvisc	0.0002591	Paxs	559.43	Joback Method
dvisc	0.0001582	Paxs	621.00	Joback Method
dvisc	0.0001056	Paxs	682.58	Joback Method
dvisc	0.0000753	Paxs	744.15	Joback Method
dvisc	0.0000566	Paxs	805.73	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=U406080&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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