

5-Phenylvaleric acid, nonyl ester

Inchi:	InChI=1S/C20H32O2/c1-2-3-4-5-6-7-13-18-22-20(21)17-12-11-16-19-14-9-8-10-15-19/h
InchiKey:	LDJNXWXWSPXLJO-UHFFFAOYSA-N
Formula:	C20H32O2
SMILES:	CCCCCCCCCOC(=O)CCCCc1ccccc1
Mol. weight [g/mol]:	304.47

Physical Properties

Property code	Value	Unit	Source
gf	-3.99	kJ/mol	Joback Method
hf	-464.40	kJ/mol	Joback Method
hfus	44.38	kJ/mol	Joback Method
hvap	71.55	kJ/mol	Joback Method
log10ws	-6.16		Crippen Method
logp	5.693		Crippen Method
mvol	276.340	ml/mol	McGowan Method
pc	1311.80	kPa	Joback Method
rinpol	2298.00		NIST Webbook
rinpol	2298.00		NIST Webbook
tb	759.97	K	Joback Method
tc	950.54	K	Joback Method
tf	413.74	K	Joback Method
vc	1.071	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	826.21	J/molxK	759.97	Joback Method
cpg	844.50	J/molxK	791.73	Joback Method
cpg	861.73	J/molxK	823.49	Joback Method
cpg	877.96	J/molxK	855.25	Joback Method
cpg	893.22	J/molxK	887.02	Joback Method
cpg	907.53	J/molxK	918.78	Joback Method
cpg	920.95	J/molxK	950.54	Joback Method
dvisc	0.0012920	Paxs	413.74	Joback Method

dvisc	0.0005995	Paxs	471.44	Joback Method
dvisc	0.0003289	Paxs	529.15	Joback Method
dvisc	0.0002031	Paxs	586.86	Joback Method
dvisc	0.0001367	Paxs	644.56	Joback Method
dvisc	0.0000982	Paxs	702.27	Joback Method
dvisc	0.0000742	Paxs	759.97	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=U406078&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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