

5-Phenylvaleric acid, octyl ester

Inchi:	InChI=1S/C19H30O2/c1-2-3-4-5-6-12-17-21-19(20)16-11-10-15-18-13-8-7-9-14-18/h7-9,
InchiKey:	FKKIRYZQILFFFD-UHFFFAOYSA-N
Formula:	C19H30O2
SMILES:	CCCCCCCCOC(=O)CCCCc1ccccc1
Mol. weight [g/mol]:	290.44

Physical Properties

Property code	Value	Unit	Source
gf	-12.41	kJ/mol	Joback Method
hf	-443.76	kJ/mol	Joback Method
hfus	41.79	kJ/mol	Joback Method
hvap	69.32	kJ/mol	Joback Method
log10ws	-5.74		Crippen Method
logp	5.303		Crippen Method
mvol	262.250	ml/mol	McGowan Method
pc	1408.01	kPa	Joback Method
rinpol	2197.00		NIST Webbook
rinpol	2197.00		NIST Webbook
tb	737.09	K	Joback Method
tc	928.11	K	Joback Method
tf	402.47	K	Joback Method
vc	1.016	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	768.05	J/molxK	737.09	Joback Method
cpg	786.09	J/molxK	768.93	Joback Method
cpg	803.11	J/molxK	800.76	Joback Method
cpg	819.14	J/molxK	832.60	Joback Method
cpg	834.22	J/molxK	864.43	Joback Method
cpg	848.38	J/molxK	896.27	Joback Method
cpg	861.65	J/molxK	928.11	Joback Method
dvisc	0.0014187	Paxs	402.47	Joback Method

dvisc	0.0006659	Paxs	458.24	Joback Method
dvisc	0.0003683	Paxs	514.01	Joback Method
dvisc	0.0002288	Paxs	569.78	Joback Method
dvisc	0.0001547	Paxs	625.55	Joback Method
dvisc	0.0001115	Paxs	681.32	Joback Method
dvisc	0.0000845	Paxs	737.09	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=U406077&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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