

5-Phenylvaleric acid, pentyl ester

Inchi:	InChI=1S/C16H24O2/c1-2-3-9-14-18-16(17)13-8-7-12-15-10-5-4-6-11-15/h4-6,10-11H,2
InchiKey:	PFGACVOYKHVCPJ-UHFFFAOYSA-N
Formula:	C16H24O2
SMILES:	CCCCCOC(=O)CCCCc1ccccc1
Mol. weight [g/mol]:	248.36

Physical Properties

Property code	Value	Unit	Source
gf	-37.67	kJ/mol	Joback Method
hf	-381.84	kJ/mol	Joback Method
hfus	34.02	kJ/mol	Joback Method
hvap	62.64	kJ/mol	Joback Method
log10ws	-4.49		Crippen Method
logp	4.133		Crippen Method
mvol	219.980	ml/mol	McGowan Method
pc	1769.87	kPa	Joback Method
rinpol	1843.00		NIST Webbook
rinpol	1843.00		NIST Webbook
tb	668.45	K	Joback Method
tc	863.72	K	Joback Method
tf	368.66	K	Joback Method
vc	0.848	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	599.99	J/molxK	668.45	Joback Method
cpg	617.16	J/molxK	701.00	Joback Method
cpg	633.37	J/molxK	733.54	Joback Method
cpg	648.65	J/molxK	766.09	Joback Method
cpg	663.03	J/molxK	798.63	Joback Method
cpg	676.54	J/molxK	831.18	Joback Method
cpg	689.21	J/molxK	863.72	Joback Method
dvisc	0.0018111	Paxs	368.66	Joback Method

dvisc	0.0008831	Paxs	418.62	Joback Method
dvisc	0.0005018	Paxs	468.59	Joback Method
dvisc	0.0003180	Paxs	518.55	Joback Method
dvisc	0.0002183	Paxs	568.52	Joback Method
dvisc	0.0001593	Paxs	618.48	Joback Method
dvisc	0.0001218	Paxs	668.45	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406073&Units=SI
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

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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