

5-Phenylvaleric acid, phenyl ester

Inchi:	InChI=1S/C17H18O2/c18-17(19-16-12-5-2-6-13-16)14-8-7-11-15-9-3-1-4-10-15/h1-6,9-1
InchiKey:	QGHHZJILQNWGDF-UHFFFAOYSA-N
Formula:	C17H18O2
SMILES:	O=C(CCCCc1ccccc1)Oc1ccccc1
Mol. weight [g/mol]:	254.32

Physical Properties

Property code	Value	Unit	Source
gf	83.16	kJ/mol	Joback Method
hf	-165.95	kJ/mol	Joback Method
hfus	30.66	kJ/mol	Joback Method
hvap	67.14	kJ/mol	Joback Method
log10ws	-4.66		Crippen Method
logp	4.005		Crippen Method
mvol	210.310	ml/mol	McGowan Method
pc	2179.52	kPa	Joback Method
rinpol	2106.00		NIST Webbook
rinpol	2106.00		NIST Webbook
tb	718.01	K	Joback Method
tc	946.64	K	Joback Method
tf	406.35	K	Joback Method
vc	0.795	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	572.19	J/molxK	718.01	Joback Method
cpg	642.51	J/molxK	908.53	Joback Method
cpg	630.71	J/molxK	870.43	Joback Method
cpg	617.83	J/molxK	832.32	Joback Method
cpg	603.83	J/molxK	794.22	Joback Method
cpg	588.63	J/molxK	756.11	Joback Method
cpg	653.31	J/molxK	946.64	Joback Method
dvisc	0.0001091	Paxs	718.01	Joback Method

dvisc	0.0001407	Paxs	666.07	Joback Method
dvisc	0.0001896	Paxs	614.12	Joback Method
dvisc	0.0002698	Paxs	562.18	Joback Method
dvisc	0.0004126	Paxs	510.24	Joback Method
dvisc	0.0006949	Paxs	458.29	Joback Method
dvisc	0.0013370	Paxs	406.35	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406898&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

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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