5-Phenylvaleric acid

Other names:	5-Phenylpentanoic acid
	Benzenepentanoic-acid-
	Phenylpentanoic acid
	Phenylvaleric acid
	Valeric acid, 5-phenyl-
	«delta»-Phenylvaleric acid
	Â«deltaÂ»-Phenylvaleric acid
Inchi:	InChI=1S/C11H14O2/c12-11(13)9-5-4-8-10-6-2-1-3-7-10/h1-3,6-7H,4-5,8-9H2,(H,12,13)
InchiKey:	BYHDDXPKOZIZRV-UHFFFAOYSA-N
Formula:	C11H14O2
SMILES:	O=C(O)CCCCc1ccccc1
Mol. weight [g/mol]:	178.23
CAS:	2270-20-4

Physical Properties

Property code	Value	Unit	Source
gf	-111.59	kJ/mol	Joback Method
hf	-298.65	kJ/mol	Joback Method
hfus	23.97	kJ/mol	Joback Method
hsub	119.40 ± 1.10	kJ/mol	NIST Webbook
hvap	65.78	kJ/mol	Joback Method
log10ws	-2.63		Crippen Method
logp	2.484		Crippen Method
mcvol	149.530	ml/mol	McGowan Method
pc	2950.00	kPa	Critical-Point Measurements for Phenylethanoic to 7-Phenylheptanoic Acids
tb	623.81	K	Joback Method
tc	821.40	K	Joback Method
tf	350.90	K	Joback Method
vc	0.569	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	437.50	J/mol×K	821.40	Joback Method
cpg	375.55	J/mol×K	623.81	Joback Method
cpg	387.56	J/mol×K	656.74	Joback Method
cpg	398.85	J/mol×K	689.67	Joback Method
cpg	409.46	J/mol×K	722.61	Joback Method
cpg	419.42	J/mol×K	755.54	Joback Method
cpg	428.76	J/mol×K	788.47	Joback Method
dvisc	0.0000781	Pa×s	623.81	Joback Method
dvisc	0.0050612	Pa×s	350.90	Joback Method
dvisc	0.0016949	Pa×s	396.38	Joback Method
dvisc	0.0007109	Pa×s	441.87	Joback Method
dvisc	0.0003507	Pa×s	487.36	Joback Method
dvisc	0.0001952	Pa×s	532.84	Joback Method
dvisc	0.0001191	Pa×s	578.32	Joback Method
hfust	23.40	kJ/mol	332.00	NIST Webbook
hsubt	118.50 ± 0.80	kJ/mol	321.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	450.70	K	1.70	NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Critical-Point Measurements for Phenylethanoic to 7-Phenylheptanoic Acids: https://www.doi.org/10.1021/je060078g

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=C2270204&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume