6-Phenylhexanoic acid

Other names: Benzenehexanoic acid
Inchi: InChI=1S/C12H16O2/c13-12(14)10-6-2-5-9-11-7-3-1-4-8-11/h1,3-4,7-8H,2,5-6,9-10H2,(H
InchiKey: JTXZPQIXIXYMDY-UHFFFAOYSA-N
Formula: C12H16O2
SMILES: O=C(O)CCCCCc1ccccc1
Mol. weight [g/mol]: 192.25
CAS: 5581-75-9

Physical Properties

Property code	Value	Unit	Source
gf	-103.17	kJ/mol	Joback Method
hf	-319.29	kJ/mol	Joback Method
hfus	26.56	kJ/mol	Joback Method
hvap	68.01	kJ/mol	Joback Method
log10ws	-3.05		Crippen Method
logp	2.874		Crippen Method
mcvol	163.620	ml/mol	McGowan Method
pc	2600.00	kPa	Critical-Point Measurements for Phenylethanoic to 7-Phenylheptanoic Acids
tb	646.69	K	Joback Method
tc	841.89	K	Joback Method
tf	362.17	K	Joback Method
vc	0.625	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	424.96	J/mol×K	646.69	Joback Method
cpg	437.59	J/mol×K	679.22	Joback Method
cpg	449.48	J/mol×K	711.76	Joback Method
cpg	460.66	J/mol×K	744.29	Joback Method
cpg	471.16	J/mol×K	776.82	Joback Method
cpg	481.02	J/mol×K	809.36	Joback Method

cpg	490.27	J/mol×K	841.89	Joback Method
dvisc	0.0043132	Pa×s	362.17	Joback Method
dvisc	0.0014364	Pa×s	409.59	Joback Method
dvisc	0.0006010	Pa×s	457.01	Joback Method
dvisc	0.0002962	Pa×s	504.43	Joback Method
dvisc	0.0001649	Pa×s	551.85	Joback Method
dvisc	0.0001007	Pa×s	599.27	Joback Method
dvisc	0.0000661	Pa×s	646.69	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	474.70	K	3.20	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=C5581759&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
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