Hexanoic acid, 4-phenyl-

Inchi: InChI=1S/C12H16O2/c1-2-10(8-9-12(13)14)11-6-4-3-5-7-11/h3-7,10H,2,8-9H2,1H3,(H,13
InchiKey: UDMXQDPTPVIQAG-UHFFFAOYSA-N
Formula: C12H16O2
SMILES: CCC(CCC(=O)O)c1ccccc1
Mol. weight [g/mol]: 192.25
CAS: 5354-04-1

Physical Properties

Property code	Value	Unit	Source
gf	-105.61	kJ/mol	Joback Method
hf	-324.57	kJ/mol	Joback Method
hfus	23.04	kJ/mol	Joback Method
hvap	67.62	kJ/mol	Joback Method
log10ws	-3.01		Crippen Method
logp	3.045		Crippen Method
mcvol	163.620	ml/mol	McGowan Method
pc	2841.41	kPa	Joback Method
tb	646.25	K	Joback Method
tc	844.92	K	Joback Method
tf	347.17	K	Joback Method
vc	0.619	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	425.46	J/mol×K	646.25	Joback Method
cpg	438.35	J/mol×K	679.36	Joback Method
cpg	450.47	J/mol×K	712.47	Joback Method
cpg	461.84	J/mol×K	745.58	Joback Method
cpg	472.50	J/mol×K	778.69	Joback Method
cpg	482.49	J/mol×K	811.81	Joback Method
cpg	491.84	J/mol×K	844.92	Joback Method
dvisc	0.0063405	Pa×s	347.17	Joback Method
dvisc	0.0018029	Pa×s	397.02	Joback Method

dvisc	0.0006786	Pa×s	446.86	Joback Method
dvisc	0.0003108	Pa×s	496.71	Joback Method
dvisc	0.0001641	Pa×s	546.56	Joback Method
dvisc	0.0000964	Pa×s	596.40	Joback Method
dvisc	0.0000615	Pa×s	646.25	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5354041&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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