

Hexanoic acid, phenyl ester

Other names:	Phenyl caproate Phenyl hexanoate
Inchi:	InChI=1S/C12H16O2/c1-2-3-5-10-12(13)14-11-8-6-4-7-9-11/h4,6-9H,2-3,5,10H2,1H3
InchiKey:	SOOXQKVMQBCEGW-UHFFFAOYSA-N
Formula:	C12H16O2
SMILES:	CCCCC(=O)Oc1ccccc1
Mol. weight [g/mol]:	192.25
CAS:	7780-16-7

Physical Properties

Property code	Value	Unit	Source
gf	-71.35	kJ/mol	Joback Method
hf	-299.28	kJ/mol	Joback Method
hfus	23.66	kJ/mol	Joback Method
hvap	53.74	kJ/mol	Joback Method
log10ws	-3.46		Crippen Method
logp	3.172		Crippen Method
mcvol	163.620	ml/mol	McGowan Method
pc	2517.59	kPa	Joback Method
rinpol	1223.00		NIST Webbook
rinpol	1223.00		NIST Webbook
rinpol	1196.00		NIST Webbook
tb	576.93	K	Joback Method
tc	782.93	K	Joback Method
tf	323.58	K	Joback Method
vc	0.624	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	394.04	J/mol×K	576.93	Joback Method
cpg	409.22	J/mol×K	611.26	Joback Method
cpg	423.55	J/mol×K	645.60	Joback Method
cpg	437.06	J/mol×K	679.93	Joback Method

cpg	449.76	J/mol×K	714.26	Joback Method
cpg	461.69	J/mol×K	748.60	Joback Method
cpg	472.86	J/mol×K	782.93	Joback Method
dvisc	0.0022442	Pa×s	323.58	Joback Method
dvisc	0.0011633	Pa×s	365.81	Joback Method
dvisc	0.0006908	Pa×s	408.03	Joback Method
dvisc	0.0004524	Pa×s	450.25	Joback Method
dvisc	0.0003185	Pa×s	492.48	Joback Method
dvisc	0.0002371	Pa×s	534.70	Joback Method
dvisc	0.0001842	Pa×s	576.93	Joback Method

Sources

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=C7780167&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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