Heptanophenone

Other names: n-Heptanophenone
1-Heptanone, 1-phenyl-
1-Phenylheptan-1-one
Inchi: InChI=1S/C13H18O/c1-2-3-4-8-11-13(14)12-9-6-5-7-10-12/h5-7,9-10H,2-4,8,11H2,1H3
InchiKey: UXMQORVHJMUQFD-UHFFFAOYSA-N
Formula: C13H18O
SMILES: CCCCCCC(=O)c1ccccc1
Mol. weight [g/mol]: 190.28
CAS: 1671-75-6

Physical Properties

Property code	Value	Unit	Source
gf	42.07	kJ/mol	Joback Method
hf	-187.70	kJ/mol	Joback Method
hfus	25.07	kJ/mol	Joback Method
hvap	53.55	kJ/mol	Joback Method
log10ws	-4.22		Crippen Method
logp	3.840		Crippen Method
mcvol	171.840	ml/mol	McGowan Method
pc	2329.27	kPa	Joback Method
rinpol	1538.00		NIST Webbook
rinpol	1538.00		NIST Webbook
tb	577.39	K	Joback Method
tc	782.30	K	Joback Method
tf	290.00 ± 3.00	K	NIST Webbook
vc	0.661	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	416.88	J/mol×K	577.39	Joback Method
cpg	433.07	J/mol×K	611.54	Joback Method
cpg	448.32	J/mol×K	645.69	Joback Method
cpg	462.68	J/mol×K	679.84	Joback Method

cpg	476.17	J/mol×K	713.99	Joback Method
cpg	488.84	J/mol×K	748.15	Joback Method
cpg	500.72	J/mol×K	782.30	Joback Method
dvisc	0.0029900	Pa×s	312.62	Joback Method
dvisc	0.0014586	Pa×s	356.75	Joback Method
dvisc	0.0008333	Pa×s	400.88	Joback Method
dvisc	0.0005320	Pa×s	445.00	Joback Method
dvisc	0.0003683	Pa×s	489.13	Joback Method
dvisc	0.0002710	Pa×s	533.26	Joback Method
dvisc	0.0002089	Pa×s	577.39	Joback Method
hvapt	64.60	kJ/mol	461.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	428.20	K	2.00	NIST Webbook

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1671756&Units=SI

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
hvapt: Enthalpy of vaporization at a given temperature
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume