3-Pentadecanone

Inchi: InChI=1S/C15H30O/c1-3-5-6-7-8-9-10-11-12-13-14-15(16)4-2/h3-14H2,1-2H3
InchiKey: YELXTWKVTZTDCM-UHFFFAOYSA-N
Formula: C15H30O
SMILES: CCCCCCCCCCCCC(=O)CC
Mol. weight [g/mol]: 226.40
CAS: 18787-66-1

Physical Properties

Property code	Value	Unit	Source
gf	-53.50	kJ/mol	Joback Method
hf	-465.51	kJ/mol	Joback Method
hfus	36.20	kJ/mol	Joback Method
hvap	55.73	kJ/mol	Joback Method
log10ws	-5.38		Crippen Method
logp	5.277		Crippen Method
mcvol	223.780	ml/mol	McGowan Method
pc	1485.00	kPa	Joback Method
rinpol	1675.00		NIST Webbook
rinpol	1668.00		NIST Webbook
ripol	1955.00		NIST Webbook
tb	596.47	K	Joback Method
tc	763.83	K	Joback Method
tf	308.74	K	Joback Method
vc	0.881	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	590.56	J/mol×K	596.47	Joback Method
cpg	671.69	J/mol×K	735.93	Joback Method
cpg	656.87	J/mol×K	708.04	Joback Method
cpg	641.36	J/mol×K	680.15	Joback Method
cpg	625.16	J/mol×K	652.26	Joback Method
cpg	608.23	J/mol×K	624.36	Joback Method

cpg	685.85	J/mol×K	763.83	Joback Method
dvisc	0.0001743	Pa×s	596.47	Joback Method
dvisc	0.0002327	Pa×s	548.52	Joback Method
dvisc	0.0003282	Pa×s	500.56	Joback Method
dvisc	0.0004978	Pa×s	452.61	Joback Method
dvisc	0.0008337	Pa×s	404.65	Joback Method
dvisc	0.0016037	Pa×s	356.69	Joback Method
dvisc	0.0037799	Pa×s	308.74	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.52290e+01
Coeff. B	-4.96312e+03
Coeff. C	-9.84280e+01
Temperature range (K), min.	430.60
Temperature range (K), max.	598.87

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=C18787661&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume