

6-Pentadecanone

Other names:	pentadecan-6-one
Inchi:	InChI=1S/C15H30O/c1-3-5-7-8-9-10-12-14-15(16)13-11-6-4-2/h3-14H2,1-2H3
InchiKey:	YSHXMTRDMDYAEC-UHFFFAOYSA-N
Formula:	C15H30O
SMILES:	CCCCCCCCC(=O)CCCCC
Mol. weight [g/mol]:	226.40
CAS:	1001-45-2

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
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/molxK	596.47	Joback Method
cpg	608.23	J/molxK	624.36	Joback Method
cpg	625.16	J/molxK	652.26	Joback Method
cpg	641.36	J/molxK	680.15	Joback Method
cpg	656.87	J/molxK	708.04	Joback Method
cpg	671.69	J/molxK	735.93	Joback Method
cpg	685.85	J/molxK	763.83	Joback Method
dvisc	0.0037799	Paxs	308.74	Joback Method

dvisc	0.0016037	Paxs	356.69	Joback Method
dvisc	0.0008337	Paxs	404.65	Joback Method
dvisc	0.0004978	Paxs	452.61	Joback Method
dvisc	0.0003282	Paxs	500.56	Joback Method
dvisc	0.0002327	Paxs	548.52	Joback Method
dvisc	0.0001743	Paxs	596.47	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1001452&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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