2-Tetradecanone

Other names: tetradecan-2-one
Inchi: InChI=1S/C14H28O/c1-3-4-5-6-7-8-9-10-11-12-13-14(2)15/h3-13H2,1-2H3
InchiKey: POQLVOYRGNFGRM-UHFFFAOYSA-N
Formula: C14H28O
SMILES: CCCCCCCCCCCCC(C)=O
Mol. weight [g/mol]: 212.37
CAS: 2345-27-9

Physical Properties

Property code	Value	Unit	Source
gf	-61.92	kJ/mol	Joback Method
hf	-444.87	kJ/mol	Joback Method
hfus	33.61	kJ/mol	Joback Method
hsub	130.90 ± 0.50	kJ/mol	NIST Webbook
hvap	82.10 ± 0.60	kJ/mol	NIST Webbook
log10ws	-4.96		Crippen Method
logp	4.886		Crippen Method
mcvol	209.690	ml/mol	McGowan Method
pc	1601.28	kPa	Joback Method
rhoc	237.86 ± 6.37	kg/m3	NIST Webbook
rinpol	1569.00		NIST Webbook
rinpol	1578.00		NIST Webbook
rinpol	1594.00		NIST Webbook
rinpol	1580.00		NIST Webbook
rinpol	1597.00		NIST Webbook
rinpol	1600.00		NIST Webbook
rinpol	1580.00		NIST Webbook
rinpol	1570.00		NIST Webbook
rinpol	271.41		NIST Webbook
rinpol	1576.00		NIST Webbook
rinpol	1569.00		NIST Webbook
rinpol	1595.00		NIST Webbook
rinpol	1576.00		NIST Webbook
rinpol	1570.00		NIST Webbook
rinpol	1594.00		NIST Webbook
rinpol	1597.00		NIST Webbook
rinpol	1595.00		NIST Webbook

rinpol	1594.00		NIST Webbook
ripol	1855.00		NIST Webbook
ripol	1893.00		NIST Webbook
ripol	1878.00		NIST Webbook
ripol	1893.00		NIST Webbook
ripol	1907.00		NIST Webbook
ripol	1874.00		NIST Webbook
tb	573.59	K	Joback Method
tc	727.70 ± 4.80	K	NIST Webbook
tf	306.70 ± 0.10	K	NIST Webbook
vc	0.826	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	630.18	J/mol×K	741.67	Joback Method
cpg	601.98	J/mol×K	685.64	Joback Method
cpg	586.91	J/mol×K	657.63	Joback Method
cpg	571.17	J/mol×K	629.62	Joback Method
cpg	554.73	J/mol×K	601.60	Joback Method
cpg	537.57	J/mol×K	573.59	Joback Method
cpg	616.40	J/mol×K	713.66	Joback Method
cps	415.20	J/mol×K	298.15	NIST Webbook
dvisc	0.0017253	Pa×s	343.49	Joback Method
dvisc	0.0009053	Pa×s	389.51	Joback Method
dvisc	0.0005444	Pa×s	435.53	Joback Method
dvisc	0.0003608	Pa×s	481.55	Joback Method
dvisc	0.0002569	Pa×s	527.57	Joback Method
dvisc	0.0040142	Pa×s	297.47	Joback Method
dvisc	0.0001932	Pa×s	573.59	Joback Method
hfust	49.12	kJ/mol	306.70	NIST Webbook
hfust	49.12	kJ/mol	306.70	NIST Webbook
hfust	49.12	kJ/mol	306.70	NIST Webbook
hvapt	64.40	kJ/mol	461.50	NIST Webbook
hvapt	55.60	kJ/mol	596.00	NIST Webbook
hvapt	65.60	kJ/mol	485.50	NIST Webbook
hvapt	51.60	kJ/mol	527.50	NIST Webbook
sfust	160.20	J/mol×K	306.70	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	478.70	K	13.30	NIST Webbook
tbrp	407.20	K	1.70	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.52533e+01
Coeff. B	-4.84963e+03
Coeff. C	-9.43700e+01
Temperature range (K), min.	418.42
Temperature range (K), max.	582.17

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=C2345279&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

cps: Solid phase 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
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation 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
pvap:	Vapor pressure
rhoc:	Critical density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume