3-Tetradecanone

Other names: tetradecan-3-one
Inchi: InChI=1S/C14H28O/c1-3-5-6-7-8-9-10-11-12-13-14(15)4-2/h3-13H2,1-2H3
InchiKey: OCHYRSKMMMYUMI-UHFFFAOYSA-N
Formula: C14H28O
SMILES: CCCCCCCCCCCC(=O)CC
Mol. weight [g/mol]: 212.37
CAS: 629-23-2

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
hvap	53.50	kJ/mol	Joback Method
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	1568.00		NIST Webbook
rinpol	1568.00		NIST Webbook
rinpol	1585.00		NIST Webbook
rinpol	1585.00		NIST Webbook
rinpol	1573.00		NIST Webbook
ripol	1855.00		NIST Webbook
ripol	1855.00		NIST Webbook
tb	573.59	K	Joback Method
tc	726.80 ± 3.70	K	NIST Webbook
tf	297.47	K	Joback Method
vc	0.826	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	537.57	J/mol×K	573.59	Joback Method
cpg	554.73	J/mol×K	601.60	Joback Method
cpg	571.17	J/mol×K	629.62	Joback Method
cpg	586.91	J/mol×K	657.63	Joback Method
cpg	601.98	J/mol×K	685.64	Joback Method
cpg	616.40	J/mol×K	713.66	Joback Method
cpg	630.18	J/mol×K	741.67	Joback Method
dvisc	0.0040142	Pa×s	297.47	Joback Method
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	0.0001932	Pa×s	573.59	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	425.20	K	2.10	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.53929e+01
Coeff. B	-4.91033e+03
Coeff. C	-9.46480e+01
Temperature range (K), min.	419.72
Temperature range (K), max.	581.71

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C629232&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/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
rhoc:	Critical density
rinpol:	Non-polar retention indices
ripol:	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