4-Tetradecanone

Other names: tetradecan-4-one
Inchi: InChI=1S/C14H28O/c1-3-5-6-7-8-9-10-11-13-14(15)12-4-2/h3-13H2,1-2H3
InchiKey: OWIOJZLDFONFSU-UHFFFAOYSA-N
Formula: C14H28O
SMILES: CCCCCCCCCCC(=O)CCC
Mol. weight [g/mol]: 212.37
CAS: 26496-20-8

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	235.73 ± 6.37	kg/m3	NIST Webbook
tb	573.59	K	Joback Method
tc	725.20 ± 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

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.52122e+01
Coeff. B	-4.83443e+03
Coeff. C	-9.40360e+01
Temperature range (K), min.	417.96
Temperature range (K), max.	582.33

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C26496208&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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume