3-Tridecanone

Other names: tridecan-3-one
Inchi: InChI=1S/C13H26O/c1-3-5-6-7-8-9-10-11-12-13(14)4-2/h3-12H2,1-2H3
InchiKey: ZDIXOWNDGFVYNK-UHFFFAOYSA-N
Formula: C13H26O
SMILES: CCCCCCCCCCC(=O)CC
Mol. weight [g/mol]: 198.34
CAS: 1534-26-5

Physical Properties

Property code	Value	Unit	Source
gf	-70.34	kJ/mol	Joback Method
hf	-424.23	kJ/mol	Joback Method
hfus	31.02	kJ/mol	Joback Method
hvap	51.28	kJ/mol	Joback Method
log10ws	-4.54		Crippen Method
logp	4.496		Crippen Method
mcvol	195.600	ml/mol	McGowan Method
pc	1731.78	kPa	Joback Method
rhoc	241.98 ± 7.93	kg/m3	NIST Webbook
rinpol	1467.00		NIST Webbook
rinpol	1467.00		NIST Webbook
rinpol	1472.00		NIST Webbook
rinpol	1498.00		NIST Webbook
rinpol	1498.00		NIST Webbook
ripol	1755.00		NIST Webbook
tb	550.71	K	Joback Method
tc	716.10 ± 1.70	K	NIST Webbook
tf	286.20	K	Joback Method
vc	0.769	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	486.12	J/mol×K	550.71	Joback Method

cpg	502.70	J/mol×K	578.88	Joback Method
cpg	518.60	J/mol×K	607.06	Joback Method
cpg	533.84	J/mol×K	635.23	Joback Method
cpg	548.43	J/mol×K	663.40	Joback Method
cpg	562.38	J/mol×K	691.58	Joback Method
cpg	575.73	J/mol×K	719.75	Joback Method
dvisc	0.0042194	Pa×s	286.20	Joback Method
dvisc	0.0018390	Pa×s	330.28	Joback Method
dvisc	0.0009747	Pa×s	374.37	Joback Method
dvisc	0.0005905	Pa×s	418.46	Joback Method
dvisc	0.0003936	Pa×s	462.54	Joback Method
dvisc	0.0002816	Pa×s	506.62	Joback Method
dvisc	0.0002125	Pa×s	550.71	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	413.20	K	2.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.56282e+01
Coeff. B	-4.87724e+03
Coeff. C	-9.08450e+01
Temperature range (K), min.	408.78
Temperature range (K), max.	563.60

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=C1534265&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
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