12-Tricosanone

Other names:	Diundecyl ketone
	Lauron
	Laurone
	Undecyl ketone
	di-n-Undecyl ketone
	tricosan-12-one
Inchi:	InChI=1S/C23H46O/c1-3-5-7-9-11-13-15-17-19-21-23(24)22-20-18-16-14-12-10-8-6-4-2/
InchiKey:	VARQGBHBYZTYLJ-UHFFFAOYSA-N
Formula:	C23H46O
SMILES:	CCCCCCCCCCCC(=O)CCCCCCCCCCC
Mol. weight [g/mol]:	338.61
CAS:	540-09-0

Physical Properties

Property code	Value	Unit	Source
gf	13.86	kJ/mol	Joback Method
hf	-630.63	kJ/mol	Joback Method
hfus	56.92	kJ/mol	Joback Method
hvap	73.54	kJ/mol	Joback Method
log10ws	-8.73		Crippen Method
logp	8.397		Crippen Method
mcvol	336.500	ml/mol	McGowan Method
pc	884.19	kPa	Joback Method
tb	779.51	K	Joback Method
tc	956.06	K	Joback Method
tf	342.00 ± 0.50	K	NIST Webbook
vc	1.329	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1155.46	J/mol×K	926.63	Joback Method
cpg	1138.14	J/mol×K	897.21	Joback Method
cpg	1119.90	J/mol×K	867.78	Joback Method

cpg	1100.72	J/mol×K	838.36	Joback Method
cpg	1080.54	J/mol×K	808.93	Joback Method
cpg	1059.34	J/mol×K	779.51	Joback Method
cpg	1171.91	J/mol×K	956.06	Joback Method
dvisc	0.0017989	Pa×s	398.90	Joback Method
dvisc	0.0000642	Pa×s	779.51	Joback Method
dvisc	0.0000875	Pa×s	716.08	Joback Method
dvisc	0.0001267	Pa×s	652.64	Joback Method
dvisc	0.0001985	Pa×s	589.20	Joback Method
dvisc	0.0003466	Pa×s	525.77	Joback Method
dvisc	0.0007053	Pa×s	462.33	Joback Method
hfust	78.03	kJ/mol	342.20	NIST Webbook
hfust	78.03	kJ/mol	342.20	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.56923e+01
Coeff. B	-6.01682e+03
Coeff. C	-1.29537e+02
Temperature range (K), min.	520.12
Temperature range (K), max.	709.15

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=C540090&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
hfust:	Enthalpy of fusion at a given temperature
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