4-Dodecanone

Other names: Octyl propyl ketone
dodecan-4-one
Inchi: InChI=1S/C12H24O/c1-3-5-6-7-8-9-11-12(13)10-4-2/h3-11H2,1-2H3
InchiKey: AVQSOIZWTINZLU-UHFFFAOYSA-N
Formula: C12H24O
SMILES: CCCCCCCCC(=O)CCC
Mol. weight [g/mol]: 184.32
CAS: 6137-26-4

Physical Properties

Property code	Value	Unit	Source
gf	-78.76	kJ/mol	Joback Method
hf	-403.59	kJ/mol	Joback Method
hfus	28.43	kJ/mol	Joback Method
hvap	49.05	kJ/mol	Joback Method
log10ws	-4.13		Crippen Method
logp	4.106		Crippen Method
mcvol	181.510	ml/mol	McGowan Method
pc	1878.90	kPa	Joback Method
rhoc	243.30 ± 7.37	kg/m3	NIST Webbook
rinpol	1367.00		NIST Webbook
tb	527.83	K	Joback Method
tc	696.60 ± 1.50	K	NIST Webbook
tf	284.65 ± 2.00	K	NIST Webbook
vc	0.714	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	436.30	J/mol×K	527.83	Joback Method
cpg	452.25	J/mol×K	556.19	Joback Method
cpg	467.55	J/mol×K	584.56	Joback Method
cpg	482.21	J/mol×K	612.92	Joback Method
cpg	496.25	J/mol×K	641.28	Joback Method

cpg	509.69	J/mol×K	669.65	Joback Method
cpg	522.54	J/mol×K	698.01	Joback Method
dvisc	0.0043838	Pa×s	274.93	Joback Method
dvisc	0.0019395	Pa×s	317.08	Joback Method
dvisc	0.0010391	Pa×s	359.23	Joback Method
dvisc	0.0006347	Pa×s	401.38	Joback Method
dvisc	0.0004257	Pa×s	443.53	Joback Method
dvisc	0.0003061	Pa×s	485.68	Joback Method
dvisc	0.0002319	Pa×s	527.83	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.52621e+01
Coeff. B	-4.59344e+03
Coeff. C	-8.48900e+01
Temperature range (K), min.	391.64
Temperature range (K), max.	546.51

Sources

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=C6137264&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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume