

6-Dodecanone

Inchi:	InChI=1S/C12H24O/c1-3-5-7-9-11-12(13)10-8-6-4-2/h3-11H2,1-2H3
InchiKey:	ZAQZICGOYPRHCK-UHFFFAOYSA-N
Formula:	C12H24O
SMILES:	CCCCCCC(=O)CCCCC
Mol. weight [g/mol]:	184.32
CAS:	6064-27-3

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	241.46 ± 7.37	kg/m ³	NIST Webbook
rinpol	1353.00		NIST Webbook
rinpol	1355.00		NIST Webbook
tb	527.83	K	Joback Method
tc	694.20 ± 1.20	K	NIST Webbook
tf	282.15 ± 2.00	K	NIST Webbook
tf	283.65 ± 2.00	K	NIST Webbook
tf	281.65 ± 2.00	K	NIST Webbook
vc	0.714	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	436.30	J/mol×K	527.83	Joback Method
cpg	509.69	J/mol×K	669.65	Joback Method
cpg	496.25	J/mol×K	641.28	Joback Method
cpg	482.21	J/mol×K	612.92	Joback Method

cpg	467.55	J/molxK	584.56	Joback Method
cpg	452.25	J/molxK	556.19	Joback Method
cpg	522.54	J/molxK	698.01	Joback Method
dvisc	0.0002319	Paxs	527.83	Joback Method
dvisc	0.0003061	Paxs	485.68	Joback Method
dvisc	0.0004257	Paxs	443.53	Joback Method
dvisc	0.0006347	Paxs	401.38	Joback Method
dvisc	0.0010391	Paxs	359.23	Joback Method
dvisc	0.0019395	Paxs	317.08	Joback Method
dvisc	0.0043838	Paxs	274.93	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
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:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C6064273&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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

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