

trans-3-Nonen-2-one

Other names:	(3E)-3-Nonen-2-one (E)-3-Nonen-2-one (E)-Non-3-en-2-one
Inchi:	InChI=1S/C9H16O/c1-3-4-5-6-7-8-9(2)10/h7-8H,3-6H2,1-2H3/b8-7+
InchiKey:	HDKLIZDXVUCLHQ-BQYQJAHWSA-N
Formula:	C9H16O
SMILES:	CCCCC=CC(C)=O
Mol. weight [g/mol]:	140.22
CAS:	18402-83-0

Physical Properties

Property code	Value	Unit	Source
gf	-23.80	kJ/mol	Joback Method
hf	-224.45	kJ/mol	Joback Method
hfus	20.87	kJ/mol	Joback Method
hvap	42.33	kJ/mol	Joback Method
log10ws	-2.72		Crippen Method
logp	2.712		Crippen Method
mcvol	134.940	ml/mol	McGowan Method
pc	2584.59	kPa	Joback Method
rinpol	1122.00		NIST Webbook
rinpol	1125.00		NIST Webbook
rinpol	1144.00		NIST Webbook
rinpol	1125.00		NIST Webbook
ripol	1523.00		NIST Webbook
tb	463.35	K	Joback Method
tc	645.65	K	Joback Method
tf	236.04	K	Joback Method
vc	0.525	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	281.50	J/mol×K	463.35	Joback Method

cpg	341.68	J/molxK	615.27	Joback Method
cpg	330.78	J/molxK	584.89	Joback Method
cpg	319.33	J/molxK	554.50	Joback Method
cpg	307.32	J/molxK	524.12	Joback Method
cpg	294.71	J/molxK	493.73	Joback Method
cpg	352.05	J/molxK	645.65	Joback Method
dvisc	0.0002369	Paxs	463.35	Joback Method
dvisc	0.0003089	Paxs	425.47	Joback Method
dvisc	0.0004242	Paxs	387.58	Joback Method
dvisc	0.0006239	Paxs	349.69	Joback Method
dvisc	0.0010078	Paxs	311.81	Joback Method
dvisc	0.0018590	Paxs	273.93	Joback Method
dvisc	0.0041736	Paxs	236.04	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.27643e+01
Coeff. B	-3.39561e+03
Coeff. C	-6.80630e+01
Temperature range (K), min.	340.22
Temperature range (K), max.	523.67

Sources

The Yaws Handbook of Vapor

Pressure:
Crippen Method:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

<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=C18402830&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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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