

11-dodecenal

Other names:	dodec-11-en-1-al
Inchi:	InChI=1S/C12H22O/c1-2-3-4-5-6-7-8-9-10-11-12-13/h2,12H,1,3-11H2
InchiKey:	LRLMEXPRIMROMY-UHFFFAOYSA-N
Formula:	C12H22O
SMILES:	C=CCCCCCCCCCC=O
Mol. weight [g/mol]:	182.30
CAS:	51148-68-6

Physical Properties

Property code	Value	Unit	Source
gf	38.48	kJ/mol	Joback Method
hf	-251.16	kJ/mol	Joback Method
hfus	27.84	kJ/mol	Joback Method
hvap	48.36	kJ/mol	Joback Method
log10ws	-3.98		Crippen Method
logp	3.882		Crippen Method
mcvol	177.210	ml/mol	McGowan Method
pc	1968.30	kPa	Joback Method
rinpol	1401.00		NIST Webbook
ripol	1753.00		NIST Webbook
tb	519.30	K	Joback Method
tc	688.58	K	Joback Method
tf	265.24	K	Joback Method
vc	0.706	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	417.40	J/molxK	519.30	Joback Method
cpg	432.51	J/molxK	547.51	Joback Method
cpg	446.98	J/molxK	575.73	Joback Method
cpg	460.83	J/molxK	603.94	Joback Method
cpg	474.08	J/molxK	632.16	Joback Method
cpg	486.74	J/molxK	660.37	Joback Method

cpg	498.84	J/mol×K	688.58	Joback Method
dvisc	0.0046526	Paxs	265.24	Joback Method
dvisc	0.0020620	Paxs	307.58	Joback Method
dvisc	0.0011128	Paxs	349.93	Joback Method
dvisc	0.0006861	Paxs	392.27	Joback Method
dvisc	0.0004648	Paxs	434.61	Joback Method
dvisc	0.0003374	Paxs	476.96	Joback Method
dvisc	0.0002581	Paxs	519.30	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.42287e+01
Coeff. B	-4.33600e+03
Coeff. C	-8.76980e+01
Temperature range (K), min.	398.72
Temperature range (K), max.	573.95

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=C51148686&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
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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