11-DODECEN-1-OL

Other names: dodec-11-enol
Inchi: InChI=1S/C12H24O/c1-2-3-4-5-6-7-8-9-10-11-12-13/h2,13H,1,3-12H2
InchiKey: QNXYZQSFDTZEBK-UHFFFAOYSA-N
Formula: C12H24O
SMILES: C=CCCCCCCCCCCO
Mol. weight [g/mol]: 184.32
CAS: 35289-31-7

Physical Properties

Property code	Value	Unit	Source
af	0.8114		Cheméo Relay (1.0)
gf	1.18	kJ/mol	Joback Method
hf	-339.09	kJ/mol	Cheméo Relay (1.0)
hfus	29.64	kJ/mol	Joback Method
hvap	90.80	kJ/mol	Cheméo Relay (1.0)
ie	9.57	eV	Cheméo Relay (1.0)
log10ws	-4.18		Cheméo Relay (1.0)
logp	3.676		Crippen Method
mcvol	181.510	ml/mol	McGowan Method
pc	2000.12	kPa	Joback Method
rinpol	1466.00		NIST Webbook
rinpol	1466.00		NIST Webbook
rinpol	1443.00		NIST Webbook
ripol	2023.00		NIST Webbook
ripol	2023.00		NIST Webbook
tb	543.23	K	Cheméo Relay (1.0)
tc	729.94	K	Cheméo Relay (1.0)
tf	293.25	K	Cheméo Relay (1.0)
vc	0.680	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	458.09	J/mol×K	562.82	Joback Method

cpg	472.22	J/mol×K	589.48	Joback Method
cpg	485.77	J/mol×K	616.14	Joback Method
cpg	498.77	J/mol×K	642.79	Joback Method
cpg	511.23	J/mol×K	669.45	Joback Method
cpg	523.18	J/mol×K	696.11	Joback Method
cpg	534.63	J/mol×K	722.77	Joback Method
dvisc	0.0198716	Pa×s	284.06	Joback Method
dvisc	0.0042967	Pa×s	330.52	Joback Method
dvisc	0.0013551	Pa×s	376.98	Joback Method
dvisc	0.0005505	Pa×s	423.44	Joback Method
dvisc	0.0002673	Pa×s	469.90	Joback Method
dvisc	0.0001478	Pa×s	516.36	Joback Method
dvisc	0.0000901	Pa×s	562.82	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.44974e+01
Coeff. B	-4.60063e+03
Coeff. C	-9.07560e+01
Temperature range (K), min.	414.52
Temperature range (K), max.	591.59

Sources

Cheméo Relay (1.0, beta):

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C35289317&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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