2-DODECEN-1-OL

Other names: 2-Dodecenol
dodec-2-en-1-ol
Inchi: InChI=1S/C12H24O/c1-2-3-4-5-6-7-8-9-10-11-12-13/h10-11,13H,2-9,12H2,1H3/b11-10+
InchiKey: MLRYPOCSLBIUHY-KHPPLWFESA-N
Formula: C12H24O
SMILES: CCCCCCCCC/C=C\CO
Mol. weight [g/mol]: 184.32
CAS: 69064-37-5

Physical Properties

Property code	Value	Unit	Source
af	0.7691		Cheméo Relay (1.0)
gf	-6.44	kJ/mol	Joback Method
hf	-355.71	kJ/mol	Cheméo Relay (1.0)
hfus	31.13	kJ/mol	Joback Method
hvap	88.48	kJ/mol	Cheméo Relay (1.0)
ie	9.08	eV	Cheméo Relay (1.0)
log10ws	-4.31		Cheméo Relay (1.0)
logp	3.676		Crippen Method
mcvol	181.510	ml/mol	McGowan Method
pc	2018.13	kPa	Joback Method
tb	538.08	K	Cheméo Relay (1.0)
tc	720.02	K	Cheméo Relay (1.0)
tf	273.72	K	Cheméo Relay (1.0)
vc	0.672	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	459.51	J/mol×K	570.30	Joback Method
cpg	473.74	J/mol×K	597.51	Joback Method
cpg	487.37	J/mol×K	624.72	Joback Method
cpg	500.43	J/mol×K	651.93	Joback Method
cpg	512.93	J/mol×K	679.14	Joback Method

cpg	524.90	J/mol×K	706.35	Joback Method
cpg	536.36	J/mol×K	733.56	Joback Method
dvisc	0.0209597	Pa×s	280.74	Joback Method
dvisc	0.0040712	Pa×s	329.00	Joback Method
dvisc	0.0012026	Pa×s	377.26	Joback Method
dvisc	0.0004685	Pa×s	425.52	Joback Method
dvisc	0.0002211	Pa×s	473.78	Joback Method
dvisc	0.0001199	Pa×s	522.04	Joback Method
dvisc	0.0000721	Pa×s	570.30	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=C22104810&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume