

7-Tridecanol

Inchi:	InChI=1S/C13H28O/c1-3-5-7-9-11-13(14)12-10-8-6-4-2/h13-14H,3-12H2,1-2H3
InchiKey:	KWUWHKRBPALTGJ-UHFFFAOYSA-N
Formula:	C13H28O
SMILES:	CCCCCCC(O)CCCCC
Mol. weight [g/mol]:	200.36
CAS:	927-45-7

Physical Properties

Property code	Value	Unit	Source
gf	-80.68	kJ/mol	Joback Method
hf	-469.16	kJ/mol	Joback Method
hfus	29.99	kJ/mol	Joback Method
hvap	60.82	kJ/mol	Joback Method
log10ws	-4.64		Crippen Method
logp	4.288		Crippen Method
mcvol	199.900	ml/mol	McGowan Method
pc	1786.37	kPa	Joback Method
rinpol	1568.00		NIST Webbook
rinpol	1568.00		NIST Webbook
ripol	1852.00		NIST Webbook
tb	588.58	K	Joback Method
tc	748.59	K	Joback Method
tf	282.09	K	Joback Method
vc	0.776	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	530.09	J/molxK	588.58	Joback Method
cpg	545.60	J/molxK	615.25	Joback Method
cpg	560.50	J/molxK	641.92	Joback Method
cpg	574.79	J/molxK	668.59	Joback Method
cpg	588.50	J/molxK	695.25	Joback Method
cpg	601.64	J/molxK	721.92	Joback Method

cpg	614.23	J/mol×K	748.59	Joback Method
dvisc	0.0293029	Paxs	282.09	Joback Method
dvisc	0.0048963	Paxs	333.17	Joback Method
dvisc	0.0013165	Paxs	384.25	Joback Method
dvisc	0.0004818	Paxs	435.33	Joback Method
dvisc	0.0002178	Paxs	486.42	Joback Method
dvisc	0.0001145	Paxs	537.50	Joback Method
dvisc	0.0000673	Paxs	588.58	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.56774e+01
Coeff. B	-4.99511e+03
Coeff. C	-8.95880e+01
Temperature range (K), min.	414.16
Temperature range (K), max.	571.46

Sources

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=C927457&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

Latest version available from:

<https://www.cheméo.com/cid/12-336-5/7-Tridecanol.pdf>

Generated by Cheméo on 2024-04-27 03:24:45.932129443 +0000 UTC m=+16477534.852706760.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.