2,3-Dimethyldecane

Other names: Decane, 2,3-dimethyl
Inchi: InChI=1S/C12H26/c1-5-6-7-8-9-10-12(4)11(2)3/h11-12H,5-10H2,1-4H3
InchiKey: ZCTGYLNFWOQVHV-UHFFFAOYSA-N
Formula: C12H26
SMILES: CCCCCCCC(C)C(C)C
Mol. weight [g/mol]: 170.33
CAS: 17312-44-6

Physical Properties

Property code	Value	Unit	Source
gf	45.28	kJ/mol	Joback Method
hf	-301.57	kJ/mol	Joback Method
hfus	19.79	kJ/mol	Joback Method
hvap	41.53	kJ/mol	Joback Method
log10ws	-4.36		Crippen Method
logp	4.639		Crippen Method
mcvol	179.940	ml/mol	McGowan Method
pc	1804.63	kPa	Joback Method
rinpol	1155.00		NIST Webbook
rinpol	1158.00		NIST Webbook
tb	473.08	K	Joback Method
tc	640.63	K	Joback Method
tf	196.60 ± 2.00	K	NIST Webbook
vc	0.696	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	502.54	J/mol×K	640.63	Joback Method
cpg	488.21	J/mol×K	612.70	Joback Method
cpg	473.26	J/mol×K	584.78	Joback Method
cpg	457.68	J/mol×K	556.85	Joback Method
cpg	441.45	J/mol×K	528.93	Joback Method
cpg	424.55	J/mol×K	501.00	Joback Method

cpg	406.97	J/mol×K	473.08	Joback Method
dvisc	0.0185767	Pa×s	195.00	Joback Method
dvisc	0.0001925	Pa×s	473.08	Joback Method
dvisc	0.0002726	Pa×s	426.73	Joback Method
dvisc	0.0004202	Pa×s	380.39	Joback Method
dvisc	0.0007305	Pa×s	334.04	Joback Method
dvisc	0.0015175	Pa×s	287.69	Joback Method
dvisc	0.0041744	Pa×s	241.35	Joback Method
hvapt	50.00	kJ/mol	424.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.40796e+01
Coeff. B	-3.66943e+03
Coeff. C	-9.13150e+01
Temperature range (K), min.	357.37
Temperature range (K), max.	509.81

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=C17312446&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/ci990307l

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
hvapt:	Enthalpy of vaporization at a given temperature
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume