Undecane, 2,4-dimethyl-

Other names: 2,4-Dimethylundecane
Inchi: InChI=1S/C13H28/c1-5-6-7-8-9-10-13(4)11-12(2)3/h12-13H,5-11H2,1-4H3
InchiKey: WMZNFELFMFOGCC-UHFFFAOYSA-N
Formula: C13H28
SMILES: CCCCCCCC(C)CC(C)C
Mol. weight [g/mol]: 184.36
CAS: 17312-80-0

Physical Properties

Property code	Value	Unit	Source
gf	53.70	kJ/mol	Joback Method
hf	-322.21	kJ/mol	Joback Method
hfus	22.38	kJ/mol	Joback Method
hvap	43.76	kJ/mol	Joback Method
log10ws	-4.78		Crippen Method
logp	5.029		Crippen Method
mcvol	194.030	ml/mol	McGowan Method
pc	1665.97	kPa	Joback Method
rinpol	1223.00		NIST Webbook
rinpol	1253.00		NIST Webbook
rinpol	1160.00		NIST Webbook
rinpol	1213.00		NIST Webbook
rinpol	1208.20		NIST Webbook
rinpol	1208.00		NIST Webbook
rinpol	1160.00		NIST Webbook
rinpol	1213.00		NIST Webbook
rinpol	1208.00		NIST Webbook
rinpol	1253.00		NIST Webbook
rinpol	1208.00		NIST Webbook
rinpol	1208.00		NIST Webbook
rinpol	1223.00		NIST Webbook
tb	495.96	K	Joback Method
tc	662.44	K	Joback Method
tf	205.00 ± 3.00	K	NIST Webbook
tf	204.65 ± 3.00	K	NIST Webbook
tf	202.00 ± 2.00	K	NIST Webbook
vc	0.751	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	554.93	J/mol×K	662.44	Joback Method
cpg	540.06	J/mol×K	634.69	Joback Method
cpg	524.55	J/mol×K	606.95	Joback Method
cpg	508.38	J/mol×K	579.20	Joback Method
cpg	491.53	J/mol×K	551.45	Joback Method
cpg	473.97	J/mol×K	523.71	Joback Method
cpg	455.70	J/mol×K	495.96	Joback Method
dvisc	0.0170093	Pa×s	206.27	Joback Method
dvisc	0.0001780	Pa×s	495.96	Joback Method
dvisc	0.0002527	Pa×s	447.68	Joback Method
dvisc	0.0003903	Pa×s	399.40	Joback Method
dvisc	0.0006795	Pa×s	351.12	Joback Method
dvisc	0.0014115	Pa×s	302.83	Joback Method
dvisc	0.0038696	Pa×s	254.55	Joback Method
hvapt	52.10	kJ/mol	427.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.40721e+01
Coeff. B	-3.68906e+03
Coeff. C	-9.89300e+01
Temperature range (K), min.	366.55
Temperature range (K), max.	520.02

Sources

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

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=C17312800&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
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