2,2-Dimethyldodecane

Inchi: InChI=1S/C14H30/c1-5-6-7-8-9-10-11-12-13-14(2,3)4/h5-13H2,1-4H3
InchiKey: ATWISEHEXAEGKB-UHFFFAOYSA-N
Formula: C14H30
SMILES: CCCCCCCCCCC(C)(C)C
Mol. weight [g/mol]: 198.39
CAS: 49598-54-1

Physical Properties

Property code	Value	Unit	Source
gf	69.84	kJ/mol	Joback Method
hf	-341.04	kJ/mol	Joback Method
hfus	24.60	kJ/mol	Joback Method
hvap	45.46	kJ/mol	Joback Method
log10ws	-5.44		Crippen Method
logp	5.563		Crippen Method
mcvol	208.120	ml/mol	McGowan Method
pc	1546.35	kPa	Joback Method
rinpol	1315.00		NIST Webbook
tb	516.49	K	Joback Method
tc	684.40	K	Joback Method
tf	249.96	K	Joback Method
vc	0.808	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	508.27	J/mol×K	516.49	Joback Method
cpg	527.48	J/mol×K	544.48	Joback Method
cpg	545.85	J/mol×K	572.46	Joback Method
cpg	563.41	J/mol×K	600.45	Joback Method
cpg	580.19	J/mol×K	628.43	Joback Method
cpg	596.21	J/mol×K	656.42	Joback Method
cpg	611.50	J/mol×K	684.40	Joback Method
dvisc	0.0082820	Pa×s	249.96	Joback Method

dvisc	0.0026796	Pa×s	294.38	Joback Method
dvisc	0.0011655	Pa×s	338.80	Joback Method
dvisc	0.0006148	Pa×s	383.23	Joback Method
dvisc	0.0003704	Pa×s	427.65	Joback Method
dvisc	0.0002455	Pa×s	472.07	Joback Method
dvisc	0.0001747	Pa×s	516.49	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.40042e+01
Coeff. B	-3.82680e+03
Coeff. C	-1.05430e+02
Temperature range (K), min.	384.42
Temperature range (K), max.	545.66

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R415037&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

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

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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume