2,3-Dimethyldodecane

Inchi: InChI=1S/C14H30/c1-5-6-7-8-9-10-11-12-14(4)13(2)3/h13-14H,5-12H2,1-4H3
InchiKey: QBIXLGJCVGNDBJ-UHFFFAOYSA-N
Formula: C14H30
SMILES: CCCCCCCCCC(C)C(C)C
Mol. weight [g/mol]: 198.39
CAS: 6117-98-2

Physical Properties

Property code	Value	Unit	Source
gf	62.12	kJ/mol	Joback Method
hf	-342.85	kJ/mol	Joback Method
hfus	24.97	kJ/mol	Joback Method
hvap	45.98	kJ/mol	Joback Method
log10ws	-5.20		Crippen Method
logp	5.419		Crippen Method
mcvol	208.120	ml/mol	McGowan Method
pc	1542.71	kPa	Joback Method
rinpol	1353.00		NIST Webbook
tb	518.84	K	Joback Method
tc	684.31	K	Joback Method
tf	222.60 ± 2.00	K	NIST Webbook
vc	0.807	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	608.64	J/mol×K	684.31	Joback Method
cpg	593.31	J/mol×K	656.73	Joback Method
cpg	577.31	J/mol×K	629.15	Joback Method
cpg	560.62	J/mol×K	601.58	Joback Method
cpg	543.22	J/mol×K	574.00	Joback Method
cpg	525.09	J/mol×K	546.42	Joback Method
cpg	506.22	J/mol×K	518.84	Joback Method
dvisc	0.0154332	Pa×s	217.54	Joback Method

dvisc	0.0001631	Pa×s	518.84	Joback Method
dvisc	0.0002320	Pa×s	468.62	Joback Method
dvisc	0.0003589	Pa×s	418.41	Joback Method
dvisc	0.0006256	Pa×s	368.19	Joback Method
dvisc	0.0012995	Pa×s	317.97	Joback Method
dvisc	0.0035509	Pa×s	267.76	Joback Method
hvapt	53.40	kJ/mol	452.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.41487e+01
Coeff. B	-3.95243e+03
Coeff. C	-1.05430e+02
Temperature range (K), min.	390.58
Temperature range (K), max.	552.68

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=C6117982&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