2,2-Dimethyloctadecane

Inchi: InChI=1S/C20H42/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20(2,3)4/h5-19H2,1-4H3
InchiKey: XZFFGCIQYXSUJJ-UHFFFAOYSA-N
Formula: C20H42
SMILES: CCCCCCCCCCCCCCCCCC(C)(C)C
Mol. weight [g/mol]: 282.55
CAS: 61869-06-5

Physical Properties

Property code	Value	Unit	Source
gf	120.36	kJ/mol	Joback Method
hf	-464.88	kJ/mol	Joback Method
hfus	40.14	kJ/mol	Joback Method
hvap	58.82	kJ/mol	Joback Method
log10ws	-7.95		Crippen Method
logp	7.904		Crippen Method
mcvol	292.660	ml/mol	McGowan Method
pc	1027.94	kPa	Joback Method
rinpol	1917.00		NIST Webbook
tb	653.77	K	Joback Method
tc	818.91	K	Joback Method
tf	317.58	K	Joback Method
vc	1.145	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	842.36	J/mol×K	653.77	Joback Method
cpg	863.80	J/mol×K	681.29	Joback Method
cpg	884.29	J/mol×K	708.82	Joback Method
cpg	903.87	J/mol×K	736.34	Joback Method
cpg	922.58	J/mol×K	763.87	Joback Method
cpg	940.45	J/mol×K	791.39	Joback Method
cpg	957.52	J/mol×K	818.91	Joback Method
dvisc	0.0043077	Pa×s	317.58	Joback Method

dvisc	0.0013647	Pa×s	373.61	Joback Method
dvisc	0.0005835	Pa×s	429.64	Joback Method
dvisc	0.0003035	Pa×s	485.67	Joback Method
dvisc	0.0001807	Pa×s	541.71	Joback Method
dvisc	0.0001186	Pa×s	597.74	Joback Method
dvisc	0.0000837	Pa×s	653.77	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.39733e+01
Coeff. B	-4.35101e+03
Coeff. C	-1.41050e+02
Temperature range (K), min.	458.97
Temperature range (K), max.	643.37

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360432&Units=SI

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