1-Hentriacontene

Inchi: InChI=1S/C31H62/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-29-31-30-28-26-24-22-20-18-
InchiKey: YITPJHKSILJOFQ-UHFFFAOYSA-N
Formula: C31H62
SMILES: C=CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 434.82
CAS: 18435-54-6

Physical Properties

Property code	Value	Unit	Source
af	1.2114		Cheméo Relay (1.0)
gf	297.98	kJ/mol	Joback Method
hf	-576.18	kJ/mol	Cheméo Relay (1.0)
hfus	74.77	kJ/mol	Joback Method
hvap	153.40	kJ/mol	Cheméo Relay (1.0)
ie	10.05	eV	Cheméo Relay (1.0)
log10ws	-11.32		Cheméo Relay (1.0)
logp	12.115		Crippen Method
mcvol	443.350	ml/mol	McGowan Method
pc	580.08	kPa	Joback Method
tb	670.75	K	Cheméo Relay (1.0)
tc	824.25	K	Cheméo Relay (1.0)
tf	322.83	K	Cheméo Relay (1.0)
vc	1.755	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1520.15	J/mol×K	905.36	Joback Method
cpg	1663.74	J/mol×K	1118.31	Joback Method
cpg	1643.08	J/mol×K	1082.82	Joback Method
cpg	1621.25	J/mol×K	1047.32	Joback Method
cpg	1598.14	J/mol×K	1011.83	Joback Method
cpg	1573.66	J/mol×K	976.34	Joback Method
cpg	1547.69	J/mol×K	940.85	Joback Method

dvisc	0.0000759	Pa×s	671.37	Joback Method
dvisc	0.0000225	Pa×s	905.36	Joback Method
dvisc	0.0000312	Pa×s	827.36	Joback Method
dvisc	0.0000465	Pa×s	749.36	Joback Method
dvisc	0.0009450	Pa×s	437.37	Joback Method
dvisc	0.0001411	Pa×s	593.37	Joback Method
dvisc	0.0003162	Pa×s	515.37	Joback Method
hvapt	117.70	kJ/mol	599.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.52966e+01
Coeff. B	-6.26607e+03
Coeff. C	-1.44132e+02
Temperature range (K), min.	561.62
Temperature range (K), max.	771.67

Sources

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C18435546&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

af: Acentric Factor
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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