

1-Nonatriacontene

Inchi:	InChI=1S/C39H78/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-29-31-33-35-37-39-38-36-34
InchiKey:	KNEBRZXNWZPYBZ-UHFFFAOYSA-N
Formula:	C39H78
SMILES:	C=CC
Mol. weight [g/mol]:	547.04
CAS:	61868-17-5

Physical Properties

Property code	Value	Unit	Source
gf	365.34	kJ/mol	Joback Method
hf	-722.86	kJ/mol	Joback Method
hfus	95.49	kJ/mol	Joback Method
hvap	101.74	kJ/mol	Joback Method
log10ws	-16.00		Crippen Method
logp	15.236		Crippen Method
mcvol	556.070	ml/mol	McGowan Method
pc	413.11	kPa	Joback Method
rinpol	2895.00		NIST Webbook
rinpol	3890.00		NIST Webbook
rinpol	3880.00		NIST Webbook
rinpol	2895.00		NIST Webbook
tb	1088.40	K	Joback Method
tc	1430.19	K	Joback Method
tf	527.53	K	Joback Method
vc	2.200	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2073.52	J/molxK	1088.40	Joback Method
cpg	2114.08	J/molxK	1145.37	Joback Method
cpg	2151.37	J/molxK	1202.33	Joback Method
cpg	2185.90	J/molxK	1259.30	Joback Method
cpg	2218.20	J/molxK	1316.26	Joback Method

cpg	2248.79	J/mol×K	1373.23	Joback Method
cpg	2278.19	J/mol×K	1430.19	Joback Method
dvisc	0.0002930	Paxs	527.53	Joback Method
dvisc	0.0000958	Paxs	621.01	Joback Method
dvisc	0.0000420	Paxs	714.49	Joback Method
dvisc	0.0000223	Paxs	807.97	Joback Method
dvisc	0.0000135	Paxs	901.44	Joback Method
dvisc	0.0000089	Paxs	994.92	Joback Method
dvisc	0.0000064	Paxs	1088.40	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.46684e+01
Coeff. B	-6.45423e+03
Coeff. C	-1.60812e+02
Temperature range (K), min.	609.62
Temperature range (K), max.	850.59

Sources

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=R528128&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/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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