

2-Methyltritriacontane

Inchi:

InChI=1S/C34H70/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25-26

InchiKey:

HRSSMXMUGSEGEK-UHFFFAOYSA-N

Formula:

C34H70

SMILES:

CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC(C)C

Mol. weight [g/mol]:

478.92

CAS:

66214-27-5

Physical Properties

Property code	Value	Unit	Source
gf	232.96	kJ/mol	Joback Method
hf	-750.37	kJ/mol	Joback Method
hfus	80.29	kJ/mol	Joback Method
hvap	90.89	kJ/mol	Joback Method
log10ws	-13.81		Crippen Method
logp	13.365		Crippen Method
mcvol	489.920	ml/mol	McGowan Method
pc	499.58	kPa	Joback Method
rinpol	3362.00		NIST Webbook
rinpol	3362.00		NIST Webbook
rinpol	3362.00		NIST Webbook
tb	976.88	K	Joback Method
tc	1226.77	K	Joback Method
tf	457.94	K	Joback Method
vc	1.933	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1756.03	J/mol×K	976.88	Joback Method
cpg	1787.83	J/mol×K	1018.53	Joback Method
cpg	1817.45	J/mol×K	1060.18	Joback Method
cpg	1845.07	J/mol×K	1101.83	Joback Method
cpg	1870.84	J/mol×K	1143.48	Joback Method
cpg	1894.95	J/mol×K	1185.12	Joback Method

cpg	1917.55	J/mol×K	1226.77	Joback Method
dvisc	0.0007325	Pa×s	457.94	Joback Method
dvisc	0.0002138	Pa×s	544.43	Joback Method
dvisc	0.0000875	Pa×s	630.92	Joback Method
dvisc	0.0000444	Pa×s	717.41	Joback Method
dvisc	0.0000261	Pa×s	803.90	Joback Method
dvisc	0.0000170	Pa×s	890.39	Joback Method
dvisc	0.0000119	Pa×s	976.88	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.49454e+01
Coeff. B	-5.78824e+03
Coeff. C	-1.89850e+02
Temperature range (K), min.	584.74
Temperature range (K), max.	790.67

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=R505343&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

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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