

2-Methylpentatriacontane

Inchi: InChI=1S/C36H74/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: JYIYHCHWLVGEBB-UHFFFAOYSA-N
Formula: C36H74
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC(C)C
Mol. weight [g/mol]: 506.97
CAS: 66576-73-6

Physical Properties

Property code	Value	Unit	Source
gf	249.80	kJ/mol	Joback Method
hf	-791.65	kJ/mol	Joback Method
hfus	85.47	kJ/mol	Joback Method
hvap	95.34	kJ/mol	Joback Method
log10ws	-14.65		Crippen Method
logp	14.146		Crippen Method
mcvol	518.100	ml/mol	McGowan Method
pc	459.31	kPa	Joback Method
rinpol	3562.00		NIST Webbook
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rinpol	3562.00		NIST Webbook
tb	1022.64	K	Joback Method
tc	1304.31	K	Joback Method
tf	480.48	K	Joback Method
vc	2.046	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1895.00	J/molxK	1022.64	Joback Method
cpg	1929.92	J/molxK	1069.59	Joback Method
cpg	1962.18	J/molxK	1116.53	Joback Method
cpg	1992.06	J/molxK	1163.48	Joback Method
cpg	2019.81	J/molxK	1210.42	Joback Method
cpg	2045.68	J/molxK	1257.37	Joback Method

cpg	2069.95	J/mol×K	1304.31	Joback Method
dvisc	0.0005358	Paxs	480.48	Joback Method
dvisc	0.0001564	Paxs	570.84	Joback Method
dvisc	0.0000639	Paxs	661.20	Joback Method
dvisc	0.0000324	Paxs	751.56	Joback Method
dvisc	0.0000190	Paxs	841.92	Joback Method
dvisc	0.0000123	Paxs	932.28	Joback Method
dvisc	0.0000087	Paxs	1022.64	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.48713e+01
Coeff. B	-5.85950e+03
Coeff. C	-1.95550e+02
Temperature range (K), min.	597.34
Temperature range (K), max.	808.48

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=R505338&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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