2-Methylhentriacontane

Inchi: InChI=1S/C32H66/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: XRBHKBOAKDZICV-UHFFFAOYSA-N
Formula: C32H66
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC(C)C
Mol. weight [g/mol]: 450.87
CAS: 1720-12-3

Physical Properties

Property code	Value	Unit	Source
gf	216.12	kJ/mol	Joback Method
hf	-709.09	kJ/mol	Joback Method
hfus	75.11	kJ/mol	Joback Method
hvap	86.44	kJ/mol	Joback Method
log10ws	-12.98		Crippen Method
logp	12.585		Crippen Method
mcvol	461.740	ml/mol	McGowan Method
pc	545.39	kPa	Joback Method
rinpol	3162.00		NIST Webbook
rinpol	3165.00		NIST Webbook
rinpol	3162.00		NIST Webbook
rinpol	3160.00		NIST Webbook
rinpol	3175.00		NIST Webbook
rinpol	3159.60		NIST Webbook
rinpol	3162.00		NIST Webbook
rinpol	3159.60		NIST Webbook
tb	931.12	K	Joback Method
tc	1155.67	K	Joback Method
tf	435.40	K	Joback Method
vc	1.821	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1618.39	J/mol×K	931.12	Joback Method

cpg	1647.62	J/mol×K	968.55	Joback Method
cpg	1675.03	J/mol×K	1005.97	Joback Method
cpg	1700.75	J/mol×K	1043.40	Joback Method
cpg	1724.89	J/mol×K	1080.82	Joback Method
cpg	1747.56	J/mol×K	1118.25	Joback Method
cpg	1768.88	J/mol×K	1155.67	Joback Method
dvisc	0.0009952	Pa×s	435.40	Joback Method
dvisc	0.0002905	Pa×s	518.02	Joback Method
dvisc	0.0001190	Pa×s	600.64	Joback Method
dvisc	0.0000605	Pa×s	683.26	Joback Method
dvisc	0.0000356	Pa×s	765.88	Joback Method
dvisc	0.0000232	Pa×s	848.50	Joback Method
dvisc	0.0000163	Pa×s	931.12	Joback Method
hvapt	120.90	kJ/mol	604.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.48922e+01
Coeff. B	-5.65952e+03
Coeff. C	-1.83850e+02
Temperature range (K), min.	571.37
Temperature range (K), max.	774.57

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=C1720123&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
hvapt:	Enthalpy of vaporization at a given temperature
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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