

7-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:	FLBGBXJBPLNKOK-FYWRMAATSA-N
Formula:	C31H62
SMILES:	CCCCC=CCCCCCCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]:	434.82

Physical Properties

Property code	Value	Unit	Source
gf	290.36	kJ/mol	Joback Method
hf	-565.95	kJ/mol	Joback Method
hfus	76.25	kJ/mol	Joback Method
hvap	84.56	kJ/mol	Joback Method
log10ws	-12.65		Crippen Method
logp	12.115		Crippen Method
mcvol	443.350	ml/mol	McGowan Method
pc	582.88	kPa	Joback Method
rinpol	3079.18		NIST Webbook
rinpol	3074.00		NIST Webbook
rinpol	3074.00		NIST Webbook
rinpol	3079.18		NIST Webbook
tb	912.84	K	Joback Method
tc	1126.80	K	Joback Method
tf	434.05	K	Joback Method
vc	1.752	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1523.51	J/molxK	912.84	Joback Method
cpg	1551.00	J/molxK	948.50	Joback Method
cpg	1576.98	J/molxK	984.16	Joback Method
cpg	1601.56	J/molxK	1019.82	Joback Method
cpg	1624.86	J/molxK	1055.48	Joback Method
cpg	1646.97	J/molxK	1091.14	Joback Method

cpg	1668.02	J/molxK	1126.80	Joback Method
dvisc	0.0008791	Paxs	434.05	Joback Method
dvisc	0.0002792	Paxs	513.85	Joback Method
dvisc	0.0001207	Paxs	593.65	Joback Method
dvisc	0.0000637	Paxs	673.44	Joback Method
dvisc	0.0000384	Paxs	753.24	Joback Method
dvisc	0.0000256	Paxs	833.04	Joback Method
dvisc	0.0000183	Paxs	912.84	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R282045&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
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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