9-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: LYSGEHYFDZAOAX-HTXNQAPBSA-N
Formula: C31H62
SMILES: CCCCCCCCC=CCCCCCCCCCCCCCCCCCCCCCC
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	3069.00		NIST Webbook
rinpol	3071.23		NIST Webbook
rinpol	3070.00		NIST Webbook
rinpol	3082.00		NIST Webbook
rinpol	3070.00		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/mol×K	912.84	Joback Method
cpg	1646.97	J/mol×K	1091.14	Joback Method
cpg	1624.86	J/mol×K	1055.48	Joback Method
cpg	1601.56	J/mol×K	1019.82	Joback Method
cpg	1576.98	J/mol×K	984.16	Joback Method

cpg	1551.00	J/mol×K	948.50	Joback Method
cpg	1668.02	J/mol×K	1126.80	Joback Method
dvisc	0.0000183	Pa×s	912.84	Joback Method
dvisc	0.0000256	Pa×s	833.04	Joback Method
dvisc	0.0000384	Pa×s	753.24	Joback Method
dvisc	0.0000637	Pa×s	673.44	Joback Method
dvisc	0.0001207	Pa×s	593.65	Joback Method
dvisc	0.0002792	Pa×s	513.85	Joback Method
dvisc	0.0008791	Pa×s	434.05	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R282109&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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