

2-Heneicosene (Z)

Inchi:	InChI=1S/C21H42/c1-3-5-7-9-11-13-15-17-19-21-20-18-16-14-12-10-8-6-4-2/h3,5H,4,6-2
InchiKey:	SEPFQHJECFKHGD-HYXAFXHYSA-N
Formula:	C21H42
SMILES:	CC=CCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]:	294.56

Physical Properties

Property code	Value	Unit	Source
gf	206.16	kJ/mol	Joback Method
hf	-359.55	kJ/mol	Joback Method
hfus	50.35	kJ/mol	Joback Method
hvap	62.30	kJ/mol	Joback Method
log10ws	-8.47		Crippen Method
logp	8.214		Crippen Method
mcvol	302.450	ml/mol	McGowan Method
pc	987.64	kPa	Joback Method
rinpol	2120.00		NIST Webbook
tb	684.04	K	Joback Method
tc	849.41	K	Joback Method
tf	321.35	K	Joback Method
vc	1.192	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	879.54	J/molxK	684.04	Joback Method
cpg	900.45	J/molxK	711.60	Joback Method
cpg	920.46	J/molxK	739.16	Joback Method
cpg	939.61	J/molxK	766.72	Joback Method
cpg	957.94	J/molxK	794.28	Joback Method
cpg	975.47	J/molxK	821.85	Joback Method
cpg	992.25	J/molxK	849.41	Joback Method
dvisc	0.0031008	Paxs	321.35	Joback Method
dvisc	0.0010163	Paxs	381.80	Joback Method

dvisc	0.0004519	Paxs	442.25	Joback Method
dvisc	0.0002442	Paxs	502.69	Joback Method
dvisc	0.0001506	Paxs	563.14	Joback Method
dvisc	0.0001020	Paxs	623.59	Joback Method
dvisc	0.0000740	Paxs	684.04	Joback Method

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=R205711&Units=SI
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
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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