1-Heneicosene

Other names: Heneicosene
henicosene
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/h3H,1,4-21
InchiKey: JTOGFHAZQVDOAO-UHFFFAOYSA-N
Formula: C21H42
SMILES: C=CCCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 294.56
CAS: 27400-79-9

Physical Properties

Property code	Value	Unit	Source
gf	213.78	kJ/mol	Joback Method
hf	-351.34	kJ/mol	Joback Method
hfus	48.87	kJ/mol	Joback Method
hvap	61.67	kJ/mol	Joback Method
log10ws	-8.47		Crippen Method
logp	8.214		Crippen Method
mcvol	302.450	ml/mol	McGowan Method
pc	981.46	kPa	Joback Method
rinpol	2092.00		NIST Webbook
rinpol	2119.00		NIST Webbook
rinpol	2094.00		NIST Webbook
rinpol	2088.00		NIST Webbook
rinpol	2090.00		NIST Webbook
rinpol	2080.00		NIST Webbook
rinpol	2098.00		NIST Webbook
rinpol	2090.00		NIST Webbook
rinpol	2087.00		NIST Webbook
ripol	2127.00		NIST Webbook
ripol	2167.00		NIST Webbook
ripol	2127.00		NIST Webbook
tb	676.56	K	Joback Method
tc	839.41	K	Joback Method
tf	324.67	K	Joback Method
vc	1.192	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	876.41	J/mol×K	676.56	Joback Method
cpg	897.28	J/mol×K	703.70	Joback Method
cpg	917.28	J/mol×K	730.84	Joback Method
cpg	936.42	J/mol×K	757.99	Joback Method
cpg	954.73	J/mol×K	785.13	Joback Method
cpg	972.25	J/mol×K	812.27	Joback Method
cpg	989.01	J/mol×K	839.41	Joback Method
dvisc	0.0031744	Pa×s	324.67	Joback Method
dvisc	0.0011137	Pa×s	383.32	Joback Method
dvisc	0.0005159	Pa×s	441.97	Joback Method
dvisc	0.0002862	Pa×s	500.61	Joback Method
dvisc	0.0001797	Pa×s	559.26	Joback Method
dvisc	0.0001232	Pa×s	617.91	Joback Method
dvisc	0.0000902	Pa×s	676.56	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C27400799&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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume