1-Heneicosene

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: 1599-68-4

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	2089.10		NIST Webbook
tb	676.56	K	Joback Method
tc	839.41	K	Joback Method
tf	308.70 ± 2.00	K	NIST Webbook
tf	308.70 ± 1.50	K	NIST Webbook
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
hvapt	92.80	kJ/mol	510.00	NIST Webbook

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=C1599684&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
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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume