n-heneicosa-3,6,9,12,15,18-hexaene

Inchi: InChI=1S/C21H32/c1-3-5-7-9-11-13-15-17-19-21-20-18-16-14-12-10-8-6-4-2/h5-8,11-14,
InchiKey: AMGFAFLDDFGVIQ-NWUVBWGCSA-N
Formula: C21H32
SMILES: CCC=CCC=CCC=CCC=CCC=CCC=CCC
Mol. weight [g/mol]: 284.48

Physical Properties

Property code	Value	Unit	Source
gf	607.26	kJ/mol	Joback Method
hf	226.55	kJ/mol	Joback Method
hfus	51.36	kJ/mol	Joback Method
hvap	62.09	kJ/mol	Joback Method
log10ws	-7.73		Crippen Method
logp	7.094		Crippen Method
mcvol	280.950	ml/mol	McGowan Method
pc	1171.22	kPa	Joback Method
rinpol	2025.00		NIST Webbook
rinpol	2025.00		NIST Webbook
tb	704.84	K	Joback Method
tc	893.50	K	Joback Method
tf	295.95	K	Joback Method
vc	1.091	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	769.81	J/mol×K	704.84	Joback Method
cpg	788.59	J/mol×K	736.28	Joback Method
cpg	806.44	J/mol×K	767.73	Joback Method
cpg	823.47	J/mol×K	799.17	Joback Method
cpg	839.78	J/mol×K	830.62	Joback Method
cpg	855.45	J/mol×K	862.06	Joback Method
cpg	870.60	J/mol×K	893.50	Joback Method
dvisc	0.0023871	Pa×s	295.95	Joback Method

dvisc	0.0006147	Pa×s	364.10	Joback Method
dvisc	0.0002428	Pa×s	432.25	Joback Method
dvisc	0.0001235	Pa×s	500.39	Joback Method
dvisc	0.0000739	Pa×s	568.54	Joback Method
dvisc	0.0000493	Pa×s	636.69	Joback Method
dvisc	0.0000356	Pa×s	704.84	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R396357&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