

6-Heneicosen-11-one, (Z)-

Other names:	(Z)-6-Heneicosen-11-one
Inchi:	InChI=1S/C21H40O/c1-3-5-7-9-11-13-15-17-19-21(22)20-18-16-14-12-10-8-6-4-2/h11,13
InchiKey:	YLNMHCDVFPONQ-QBFSEMIESA-N
Formula:	C21H40O
SMILES:	CCCCC=CCCC(=O)CCCCCCCCC
Mol. weight [g/mol]:	308.54
CAS:	54844-65-4

Physical Properties

Property code	Value	Unit	Source
gf	77.24	kJ/mol	Joback Method
hf	-472.13	kJ/mol	Joback Method
hfus	51.95	kJ/mol	Joback Method
hvap	69.04	kJ/mol	Joback Method
log10ws	-7.75		Crippen Method
logp	7.393		Crippen Method
mcvol	304.020	ml/mol	McGowan Method
pc	1027.94	kPa	Joback Method
rinpol	2258.00		NIST Webbook
tb	737.91	K	Joback Method
tc	912.08	K	Joback Method
tf	371.28	K	Joback Method
vc	1.198	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	912.82	J/mol×K	737.91	Joback Method
cpg	1002.74	J/mol×K	883.05	Joback Method
cpg	986.44	J/mol×K	854.02	Joback Method
cpg	969.33	J/mol×K	824.99	Joback Method
cpg	951.39	J/mol×K	795.97	Joback Method
cpg	932.57	J/mol×K	766.94	Joback Method
cpg	1018.29	J/mol×K	912.08	Joback Method

dvisc	0.0000731	Pa×s	737.91	Joback Method
dvisc	0.0000993	Pa×s	676.80	Joback Method
dvisc	0.0001435	Pa×s	615.70	Joback Method
dvisc	0.0002249	Pa×s	554.60	Joback Method
dvisc	0.0003939	Pa×s	493.49	Joback Method
dvisc	0.0008083	Pa×s	432.38	Joback Method
dvisc	0.0021015	Pa×s	371.28	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C54844654&Units=SI

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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