1-Heneicosanol

Other names:	Henicosan-1-ol
	Heneicosyl alcohol
	Heneicosanol
	henicosanol
Inchi:	InChI=1S/C21H44O/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22/h22H,2
InchiKey:	FIPPFBHCBUDBRR-UHFFFAOYSA-N
Formula:	C21H44O
SMILES:	CCCCCCCCCCCCCCCCCCCCCO
Mol. weight [g/mol]:	312.57
CAS:	15594-90-8

Physical Properties

Property code	Value	Unit	Source
gf	-10.88	kJ/mol	Joback Method
hf	-629.00	kJ/mol	Joback Method
hfus	54.23	kJ/mol	Joback Method
hvap	79.02	kJ/mol	Joback Method
log10ws	-7.88		Crippen Method
logp	7.411		Crippen Method
mcvol	312.620	ml/mol	McGowan Method
pc	1012.95	kPa	Joback Method
rinpol	2380.00		NIST Webbook
rinpol	2401.70		NIST Webbook
rinpol	2401.70		NIST Webbook
rinpol	2365.00		NIST Webbook
rinpol	2365.00		NIST Webbook
ripol	2995.00		NIST Webbook
tb	772.06	K	Joback Method
tc	945.53	K	Joback Method
tf	387.25	K	Joback Method
vc	1.230	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	988.02	J/mol×K	772.06	Joback Method
cpg	1007.87	J/mol×K	800.97	Joback Method
cpg	1026.80	J/mol×K	829.88	Joback Method
cpg	1044.84	J/mol×K	858.79	Joback Method
cpg	1062.03	J/mol×K	887.70	Joback Method
cpg	1078.41	J/mol×K	916.61	Joback Method
cpg	1094.01	J/mol×K	945.53	Joback Method
dvisc	0.0028376	Pa×s	387.25	Joback Method
dvisc	0.0006522	Pa×s	451.38	Joback Method
dvisc	0.0002161	Pa×s	515.52	Joback Method
dvisc	0.0000914	Pa×s	579.65	Joback Method
dvisc	0.0000459	Pa×s	643.79	Joback Method
dvisc	0.0000261	Pa×s	707.92	Joback Method
dvisc	0.0000163	Pa×s	772.06	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C15594908&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
ripol: Polar retention indices

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