1-Chloroeicosane

Other names: Eicosane, 1-chloro-
chloroicosane
Inchi: InChI=1S/C20H41Cl/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21/h2-20H2,
InchiKey: AFGNVSCTEXUEJE-UHFFFAOYSA-N
Formula: C20H41Cl
SMILES: CCCCCCCCCCCCCCCCCCCCCl
Mol. weight [g/mol]: 316.99
CAS: 42217-02-7

Physical Properties

Property code	Value	Unit	Source
gf	105.59	kJ/mol	Joback Method
hf	-471.87	kJ/mol	Joback Method
hfus	51.75	kJ/mol	Joback Method
hvap	120.20	kJ/mol	NIST Webbook
log10ws	-8.35		Crippen Method
logp	8.267		Crippen Method
mcvol	304.900	ml/mol	McGowan Method
pc	992.00	kPa	Joback Method
rinpol	2264.00		NIST Webbook
rinpol	2292.00		NIST Webbook
ripol	2480.00		NIST Webbook
tb	694.43	K	Joback Method
tc	860.46	K	Joback Method
tf	345.08	K	Joback Method
vc	1.204	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	988.81	J/mol×K	860.46	Joback Method
cpg	880.32	J/mol×K	694.43	Joback Method
cpg	900.50	J/mol×K	722.10	Joback Method
cpg	919.80	J/mol×K	749.77	Joback Method

cpg	938.25	J/mol×K	777.45	Joback Method
cpg	955.88	J/mol×K	805.12	Joback Method
cpg	972.72	J/mol×K	832.79	Joback Method
dvisc	0.0000868	Pa×s	694.43	Joback Method
dvisc	0.0027293	Pa×s	345.08	Joback Method
dvisc	0.0010147	Pa×s	403.31	Joback Method
dvisc	0.0004842	Pa×s	461.53	Joback Method
dvisc	0.0002728	Pa×s	519.75	Joback Method
dvisc	0.0001725	Pa×s	577.98	Joback Method
dvisc	0.0001186	Pa×s	636.20	Joback Method
hvapt	78.30	kJ/mol	582.50	NIST Webbook

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=C42217027&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
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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point

vc: Critical Volume

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