3-Chloro-6-methylheptane

Inchi: InChI=1S/C8H17Cl/c1-4-8(9)6-5-7(2)3/h7-8H,4-6H2,1-3H3
InchiKey: GMLQONWBBDPDQO-UHFFFAOYSA-N
Formula: C8H17Cl
SMILES: CCC(Cl)CCC(C)C
Mol. weight [g/mol]: 148.68

Physical Properties

Property code	Value	Unit	Source
af	0.3729		Cheméo Relay (1.0)
gf	-0.33	kJ/mol	Joback Method
hf	-261.43	kJ/mol	Cheméo Relay (1.0)
hfus	13.63	kJ/mol	Joback Method
hvap	45.17	kJ/mol	Cheméo Relay (1.0)
ie	9.91	eV	Cheméo Relay (1.0)
log10ws	-4.37		Cheméo Relay (1.0)
logp	3.440		Crippen Method
mcvol	135.820	ml/mol	McGowan Method
pc	2482.59	kPa	Joback Method
rinpol	966.00		NIST Webbook
rinpol	966.00		NIST Webbook
rinpol	966.00		NIST Webbook
tb	431.92	K	Cheméo Relay (1.0)
tc	608.20	K	Cheméo Relay (1.0)
tf	202.16	K	Cheméo Relay (1.0)
vc	0.501	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	262.83	J/mol×K	418.99	Joback Method
cpg	335.90	J/mol×K	597.64	Joback Method
cpg	325.02	J/mol×K	567.87	Joback Method
cpg	313.63	J/mol×K	538.09	Joback Method
cpg	301.74	J/mol×K	508.32	Joback Method

cpg	289.32	J/mol×K	478.54	Joback Method
cpg	276.35	J/mol×K	448.77	Joback Method
dvisc	0.0008967	Pa×s	299.42	Joback Method
dvisc	0.0002571	Pa×s	418.99	Joback Method
dvisc	0.0003572	Pa×s	379.13	Joback Method
dvisc	0.0005362	Pa×s	339.27	Joback Method
dvisc	0.0164704	Pa×s	179.84	Joback Method
dvisc	0.0017563	Pa×s	259.56	Joback Method
dvisc	0.0043901	Pa×s	219.70	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R116022&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af: Acentric Factor
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
ie: Ionization energy
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