

Octane, 2-chloro-, (S)-

Inchi:	InChI=1S/C8H17Cl/c1-3-4-5-6-7-8(2)9/h8H,3-7H2,1-2H3/t8-/m1/s1
InchiKey:	HKDCIIMOALDWHF-MRVPVSSYSA-N
Formula:	C8H17Cl
SMILES:	CCCCCCC(C)Cl
Mol. weight [g/mol]:	148.67
CAS:	16844-08-9

Physical Properties

Property code	Value	Unit	Source
gf	2.11	kJ/mol	Joback Method
hf	-229.47	kJ/mol	Joback Method
hfus	17.15	kJ/mol	Joback Method
hvap	37.40	kJ/mol	Joback Method
log10ws	-3.44		Crippen Method
logp	3.584		Crippen Method
mcvol	135.820	ml/mol	McGowan Method
pc	2462.92	kPa	Joback Method
tb	419.43	K	Joback Method
tc	594.11	K	Joback Method
tf	194.84	K	Joback Method
vc	0.526	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	262.83	J/molxK	419.43	Joback Method
cpg	275.97	J/molxK	448.54	Joback Method
cpg	288.58	J/molxK	477.66	Joback Method
cpg	300.68	J/molxK	506.77	Joback Method
cpg	312.27	J/molxK	535.88	Joback Method
cpg	323.39	J/molxK	564.99	Joback Method
cpg	334.03	J/molxK	594.11	Joback Method
dvisc	0.0088497	Paxs	194.84	Joback Method
dvisc	0.0030882	Paxs	232.27	Joback Method

dvisc	0.0014434	Paxs	269.70	Joback Method
dvisc	0.0008121	Paxs	307.13	Joback Method
dvisc	0.0005177	Paxs	344.57	Joback Method
dvisc	0.0003605	Paxs	382.00	Joback Method
dvisc	0.0002677	Paxs	419.43	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	348.20	K	3.70	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16844089&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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point

vc: Critical Volume

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