

1,1-Dichloroheptane

Inchi:	InChI=1S/C7H14Cl2/c1-2-3-4-5-6-7(8)9/h7H,2-6H2,1H3
InchiKey:	MEMYUUBNXYUWRG-UHFFFAOYSA-N
Formula:	C7H14Cl2
SMILES:	CCCCCCC(Cl)Cl
Mol. weight [g/mol]:	169.09
CAS:	821-25-0

Physical Properties

Property code	Value	Unit	Source
gf	-18.24	kJ/mol	Joback Method
hf	-224.57	kJ/mol	Joback Method
hfus	18.76	kJ/mol	Joback Method
hvap	53.50	kJ/mol	NIST Webbook
log10ws	-3.67		Crippen Method
logp	3.761		Crippen Method
mcvol	133.970	ml/mol	McGowan Method
pc	2613.74	kPa	Joback Method
tb	468.00 ± 3.00	K	NIST Webbook
tc	616.82	K	Joback Method
tf	213.49	K	Joback Method
vc	0.519	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	251.14	J/mol×K	433.98	Joback Method
cpg	304.42	J/mol×K	586.35	Joback Method
cpg	294.73	J/mol×K	555.87	Joback Method
cpg	284.57	J/mol×K	525.40	Joback Method
cpg	273.93	J/mol×K	494.93	Joback Method
cpg	262.79	J/mol×K	464.45	Joback Method
cpg	313.66	J/mol×K	616.82	Joback Method
dvisc	0.0002988	Paxs	433.98	Joback Method
dvisc	0.0003984	Paxs	397.23	Joback Method

dvisc	0.0005634	Paxs	360.48	Joback Method
dvisc	0.0008619	Paxs	323.74	Joback Method
dvisc	0.0014701	Paxs	286.99	Joback Method
dvisc	0.0029334	Paxs	250.24	Joback Method
dvisc	0.0074245	Paxs	213.49	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C821250&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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

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