Hexane, 2,5-dichloro-, (R*,S*)-

Inchi: InChI=1S/C6H12Cl2/c1-5(7)3-4-6(2)8/h5-6H,3-4H2,1-2H3/t5-,6+
InchiKey: RRFNCPBJVPQIPP-OLQVQODUSA-N
Formula: C6H12Cl2
SMILES: CC(Cl)CCC(C)Cl
Mol. weight [g/mol]: 155.06
CAS: 41761-11-9

Physical Properties

Property code	Value	Unit	Source
gf	-29.10	kJ/mol	Joback Method
hf	-209.21	kJ/mol	Joback Method
hfus	12.64	kJ/mol	Joback Method
hvap	36.94	kJ/mol	Joback Method
log10ws	-2.86		Crippen Method
logp	3.021		Crippen Method
mcvol	119.880	ml/mol	McGowan Method
pc	2915.53	kPa	Joback Method
tb	410.66	K	Joback Method
tc	599.28	K	Joback Method
tf	187.22	K	Joback Method
vc	0.458	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	212.29	J/mol×K	410.66	Joback Method
cpg	223.08	J/mol×K	442.10	Joback Method
cpg	233.37	J/mol×K	473.53	Joback Method
cpg	243.19	J/mol×K	504.97	Joback Method
cpg	252.55	J/mol×K	536.41	Joback Method
cpg	261.47	J/mol×K	567.84	Joback Method
cpg	269.95	J/mol×K	599.28	Joback Method
dvisc	0.0130601	Pa×s	187.22	Joback Method
dvisc	0.0041501	Pa×s	224.46	Joback Method

dvisc	0.0018276	Pa×s	261.70	Joback Method
dvisc	0.0009873	Pa×s	298.94	Joback Method
dvisc	0.0006113	Pa×s	336.18	Joback Method
dvisc	0.0004165	Pa×s	373.42	Joback Method
dvisc	0.0003042	Pa×s	410.66	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	382.20	K	13.00	NIST Webbook

Sources

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=C41761119&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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