

2,5-dichloro-2,5-dimethylhexane

Inchi:	InChI=1S/C8H16Cl2/c1-7(2,9)5-6-8(3,4)10/h5-6H2,1-4H3
InchiKey:	HSTAGCWQAIXJQM-UHFFFAOYSA-N
Formula:	C8H16Cl2
SMILES:	CC(C)(Cl)CCC(C)(C)Cl
Mol. weight [g/mol]:	183.12

Physical Properties

Property code	Value	Unit	Source
gf	-1.70	kJ/mol	Joback Method
hf	-257.43	kJ/mol	Joback Method
hfus	10.04	kJ/mol	Joback Method
hvap	39.58	kJ/mol	Joback Method
log10ws	-3.70		Crippen Method
logp	3.801		Crippen Method
mcvol	148.060	ml/mol	McGowan Method
pc	2445.89	kPa	Joback Method
tb	450.84	K	Joback Method
tc	651.92	K	Joback Method
tf	244.60	K	Joback Method
vc	0.559	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	297.17	J/molxK	450.84	Joback Method
cpg	312.13	J/molxK	484.35	Joback Method
cpg	326.09	J/molxK	517.87	Joback Method
cpg	339.13	J/molxK	551.38	Joback Method
cpg	351.29	J/molxK	584.89	Joback Method
cpg	362.64	J/molxK	618.40	Joback Method
cpg	373.22	J/molxK	651.92	Joback Method
dvisc	0.0104264	Paxs	244.60	Joback Method
dvisc	0.0040292	Paxs	278.97	Joback Method
dvisc	0.0019182	Paxs	313.35	Joback Method

dvisc	0.0010575	Paxs	347.72	Joback Method
dvisc	0.0006490	Paxs	382.09	Joback Method
dvisc	0.0004317	Paxs	416.47	Joback Method
dvisc	0.0003056	Paxs	450.84	Joback Method

Sources

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=T999913621&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307i

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
hvac:	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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