

1-Pentene, 1,1,5-trichloro-

Other names:	1,1-Dichloro-1-pentenyl chloride 1,1,5-Trichloro-1-pentene
Inchi:	InChI=1S/C5H7Cl3/c6-4-2-1-3-5(7)8/h3H,1-2,4H2
InchiKey:	WIBRQEFYLNRTM-UHFFFAOYSA-N
Formula:	C5H7Cl3
SMILES:	C1CCCC=C(Cl)Cl
Mol. weight [g/mol]:	173.47
CAS:	2677-33-0

Physical Properties

Property code	Value	Unit	Source
gf	27.10	kJ/mol	Joback Method
hf	-86.32	kJ/mol	Joback Method
hfus	20.19	kJ/mol	Joback Method
hvap	39.92	kJ/mol	Joback Method
log10ws	-3.22		Crippen Method
logp	3.324		Crippen Method
mvol	113.730	ml/mol	McGowan Method
pc	3257.86	kPa	Joback Method
rinpol	1110.00		NIST Webbook
rinpol	1110.00		NIST Webbook
tb	430.13	K	Joback Method
tc	632.42	K	Joback Method
tf	216.83	K	Joback Method
vc	0.444	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	183.16	J/molxK	430.13	Joback Method
cpg	191.26	J/molxK	463.85	Joback Method
cpg	198.85	J/molxK	497.56	Joback Method
cpg	205.97	J/molxK	531.28	Joback Method
cpg	212.63	J/molxK	564.99	Joback Method

cpg	218.88	J/mol×K	598.71	Joback Method
cpg	224.74	J/mol×K	632.42	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=C2677330&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

cpg:	Ideal gas heat capacity
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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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