

6-Undecanone, 5,7-dichloro (RR, SS)

Inchi:	InChI=1S/C11H20Cl2O/c1-3-5-7-9(12)11(14)10(13)8-6-4-2/h9-10H,3-8H2,1-2H3
InchiKey:	FJFNPTNEBBJNPW-UHFFFAOYSA-N
Formula:	C11H20Cl2O
SMILES:	CCCCC(Cl)C(=O)C(Cl)CCCC
Mol. weight [g/mol]:	239.18

Physical Properties

Property code	Value	Unit	Source
gf	-115.92	kJ/mol	Joback Method
hf	-424.99	kJ/mol	Joback Method
hfus	27.19	kJ/mol	Joback Method
hvap	54.82	kJ/mol	Joback Method
log10ws	-4.24		Crippen Method
logp	4.151		Crippen Method
mcvol	191.900	ml/mol	McGowan Method
pc	1942.37	kPa	Joback Method
rinpol	1484.00		NIST Webbook
rinpol	1484.00		NIST Webbook
tb	578.93	K	Joback Method
tc	767.04	K	Joback Method
tf	293.50	K	Joback Method
vc	0.744	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	451.00	J/molxK	578.93	Joback Method
cpg	516.79	J/molxK	735.69	Joback Method
cpg	504.99	J/molxK	704.34	Joback Method
cpg	492.53	J/molxK	672.99	Joback Method
cpg	479.40	J/molxK	641.63	Joback Method
cpg	465.56	J/molxK	610.28	Joback Method
cpg	527.95	J/molxK	767.04	Joback Method
dvisc	0.0002060	Paxs	578.93	Joback Method

dvisc	0.0002811	Paxs	531.36	Joback Method
dvisc	0.0004078	Paxs	483.79	Joback Method
dvisc	0.0006417	Paxs	436.22	Joback Method
dvisc	0.0011281	Paxs	388.64	Joback Method
dvisc	0.0023214	Paxs	341.07	Joback Method
dvisc	0.0060355	Paxs	293.50	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R630652&Units=SI

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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