

4-Dodecanone, 3,5-dichloro (RR, SS)

Inchi:	InChI=1S/C12H22Cl2O/c1-3-5-6-7-8-9-11(14)12(15)10(13)4-2/h10-11H,3-9H2,1-2H3
InchiKey:	WUERIFBXEDLZSQ-UHFFFAOYSA-N
Formula:	C12H22Cl2O
SMILES:	CCCCCCCC(Cl)C(=O)C(Cl)CC
Mol. weight [g/mol]:	253.21

Physical Properties

Property code	Value	Unit	Source
gf	-107.50	kJ/mol	Joback Method
hf	-445.63	kJ/mol	Joback Method
hfus	29.78	kJ/mol	Joback Method
hvap	57.05	kJ/mol	Joback Method
log10ws	-4.66		Crippen Method
logp	4.541		Crippen Method
mcvol	205.990	ml/mol	McGowan Method
pc	1787.88	kPa	Joback Method
rinpol	1600.00		NIST Webbook
rinpol	1600.00		NIST Webbook
tb	601.81	K	Joback Method
tc	787.90	K	Joback Method
tf	304.77	K	Joback Method
vc	0.799	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	500.85	J/mol×K	601.81	Joback Method
cpg	516.02	J/mol×K	632.83	Joback Method
cpg	530.44	J/mol×K	663.84	Joback Method
cpg	544.12	J/mol×K	694.86	Joback Method
cpg	557.10	J/mol×K	725.87	Joback Method
cpg	569.39	J/mol×K	756.89	Joback Method
cpg	581.03	J/mol×K	787.90	Joback Method
dvisc	0.0055360	Paxs	304.77	Joback Method

dvisc	0.0021090	Paxs	354.28	Joback Method
dvisc	0.0010179	Paxs	403.78	Joback Method
dvisc	0.0005760	Paxs	453.29	Joback Method
dvisc	0.0003647	Paxs	502.80	Joback Method
dvisc	0.0002506	Paxs	552.30	Joback Method
dvisc	0.0001831	Paxs	601.81	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=R630449&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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