3-Pentanone, 2,4-dichloro (RS, SR)

Inchi: InChI=1S/C5H8Cl2O/c1-3(6)5(8)4(2)7/h3-4H,1-2H3
InchiKey: XNTVDJIRXYIWQH-UHFFFAOYSA-N
Formula: C5H8Cl2O
SMILES: CC(Cl)C(=O)C(C)Cl
Mol. weight [g/mol]: 155.02

Physical Properties

Property code	Value	Unit	Source
gf	-166.44	kJ/mol	Joback Method
hf	-301.15	kJ/mol	Joback Method
hfus	11.65	kJ/mol	Joback Method
hvap	41.46	kJ/mol	Joback Method
log10ws	-1.73		Crippen Method
logp	1.810		Crippen Method
mcvol	107.360	ml/mol	McGowan Method
pc	3488.88	kPa	Joback Method
rinpol	872.00		NIST Webbook
rinpol	872.00		NIST Webbook
tb	441.65	K	Joback Method
tc	644.37	K	Joback Method
tf	225.88	K	Joback Method
vc	0.407	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	189.33	J/mol×K	441.65	Joback Method
cpg	228.55	J/mol×K	610.58	Joback Method
cpg	221.55	J/mol×K	576.80	Joback Method
cpg	214.14	J/mol×K	543.01	Joback Method
cpg	206.31	J/mol×K	509.22	Joback Method
cpg	198.04	J/mol×K	475.44	Joback Method
cpg	235.16	J/mol×K	644.37	Joback Method
dvisc	0.0003609	Pa×s	441.65	Joback Method

dvisc	0.0004824	Pa×s	405.69	Joback Method
dvisc	0.0006822	Pa×s	369.73	Joback Method
dvisc	0.0010396	Pa×s	333.76	Joback Method
dvisc	0.0017540	Pa×s	297.80	Joback Method
dvisc	0.0034166	Pa×s	261.84	Joback Method
dvisc	0.0082291	Pa×s	225.88	Joback Method

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=R630370&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume