

Methylenesuccinyl chloride

Other names:	2,2-methylenesuccinyl dichloride Itaconyl chloride
Inchi:	InChI=1S/C5H4Cl2O2/c1-3(5(7)9)2-4(6)8/h1-2H2
InchiKey:	CGCRIQNPIBHVCQ-UHFFFAOYSA-N
Formula:	C5H4Cl2O2
SMILES:	C=C(CC(=O)Cl)C(=O)Cl
Mol. weight [g/mol]:	166.99
CAS:	1931-60-8

Physical Properties

Property code	Value	Unit	Source
gf	-211.19	kJ/mol	Joback Method
hf	-287.53	kJ/mol	Joback Method
hfus	17.71	kJ/mol	Joback Method
hvap	48.40	kJ/mol	Joback Method
log10ws	-1.63		Crippen Method
logp	1.463		Crippen Method
mcvol	104.630	ml/mol	McGowan Method
pc	3911.14	kPa	Joback Method
tb	492.96	K	Joback Method
tc	705.49	K	Joback Method
tf	290.09	K	Joback Method
vc	0.407	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	182.19	J/mol×K	492.96	Joback Method
cpg	188.79	J/mol×K	528.38	Joback Method
cpg	194.97	J/mol×K	563.80	Joback Method
cpg	200.73	J/mol×K	599.23	Joback Method
cpg	206.11	J/mol×K	634.65	Joback Method
cpg	211.11	J/mol×K	670.07	Joback Method
cpg	215.76	J/mol×K	705.49	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	362.20	K	2.30	NIST Webbook

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=C1931608&Units=SI

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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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