

Malonyl dichloride

Other names:	Malonyl chloride Propanedioyl dichloride Malonic acid chloride Malonic acid dichloride Malonoyl chloride Malonoyl dichloride
Inchi:	InChI=1S/C3H2Cl2O2/c4-2(6)1-3(5)7/h1H2
InchiKey:	SXYFKXOFMCIXQW-UHFFFAOYSA-N
Formula:	C3H2Cl2O2
SMILES:	O=C(Cl)CC(=O)Cl
Mol. weight [g/mol]:	140.95
CAS:	1663-67-8

Physical Properties

Property code	Value	Unit	Source
gf	-307.32	kJ/mol	Joback Method
hf	-361.89	kJ/mol	Joback Method
hfus	15.12	kJ/mol	Joback Method
hvap	44.53	kJ/mol	Joback Method
log10ws	-0.94		Crippen Method
logp	0.907		Crippen Method
mcvol	80.750	ml/mol	McGowan Method
pc	4730.11	kPa	Joback Method
tb	450.64	K	Joback Method
tc	660.36	K	Joback Method
tf	283.27	K	Joback Method
vc	0.314	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	124.93	J/mol×K	450.64	Joback Method
cpg	144.88	J/mol×K	625.41	Joback Method
cpg	141.39	J/mol×K	590.46	Joback Method

cpg	137.66	J/mol×K	555.50	Joback Method
cpg	133.67	J/mol×K	520.55	Joback Method
cpg	129.44	J/mol×K	485.59	Joback Method
cpg	148.13	J/mol×K	660.36	Joback Method
dvisc	0.0004945	Pa×s	450.64	Joback Method
dvisc	0.0006095	Pa×s	422.75	Joback Method
dvisc	0.0007738	Pa×s	394.85	Joback Method
dvisc	0.0010187	Pa×s	366.95	Joback Method
dvisc	0.0014031	Pa×s	339.06	Joback Method
dvisc	0.0020466	Pa×s	311.16	Joback Method
dvisc	0.0032159	Pa×s	283.27	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	327.20	K	2.50	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1663678&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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
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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