PROPANEDIOYL 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

Physical Properties

Property code	Value	Unit	Source
af	0.4053		Cheméo Relay (1.0)
gf	-307.32	kJ/mol	Joback Method
hf	-387.14	kJ/mol	Cheméo Relay (1.0)
hfus	15.12	kJ/mol	Joback Method
hvap	36.28	kJ/mol	Cheméo Relay (1.0)
ie	10.33	eV	Cheméo Relay (1.0)
logp	0.907		Crippen Method
mcvol	80.750	ml/mol	McGowan Method
pc	4730.11	kPa	Joback Method
tb	418.78	K	Cheméo Relay (1.0)
tc	622.85	K	Cheméo Relay (1.0)
tf	278.66	K	Cheméo Relay (1.0)
vc	0.283	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	124.93	J/mol×K	450.64	Joback Method
cpg	129.44	J/mol×K	485.59	Joback Method
cpg	133.67	J/mol×K	520.55	Joback Method

cpg	137.66	J/mol×K	555.50	Joback Method
cpg	141.39	J/mol×K	590.46	Joback Method
cpg	144.88	J/mol×K	625.41	Joback Method
cpg	148.13	J/mol×K	660.36	Joback Method
dvisc	0.0032159	Pa×s	283.27	Joback Method
dvisc	0.0020466	Pa×s	311.16	Joback Method
dvisc	0.0014031	Pa×s	339.06	Joback Method
dvisc	0.0010187	Pa×s	366.95	Joback Method
dvisc	0.0007738	Pa×s	394.85	Joback Method
dvisc	0.0006095	Pa×s	422.75	Joback Method
dvisc	0.0004945	Pa×s	450.64	Joback Method

Pressure Dependent Properties

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

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1663678&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af: Acentric Factor
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
ie:	Ionization energy
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