

SUBEROYL DICHLORIDE

Other names:	Octanedioyl dichloride Suberic acid dichloride Suberoyl dichloride Suberyl chloride Suberyl dichloride
Inchi:	InChI=1S/C8H12Cl2O2/c9-7(11)5-3-1-2-4-6-8(10)12/h1-6H2
InchiKey:	PUIBKAHUQOOLSW-UHFFFAOYSA-N
Formula:	C8H12Cl2O2
SMILES:	O=C(Cl)CCCCCCC(=O)Cl
Mol. weight [g/mol]:	211.09

Physical Properties

Property code	Value	Unit	Source
hf	-514.89	kJ/mol	Cheméo Relay (1.0)
hfus	28.07	kJ/mol	Joback Method
hvap	64.04	kJ/mol	Cheméo Relay (1.0)
ie	10.01	eV	Cheméo Relay (1.0)
log10ws	-3.66		Cheméo Relay (1.0)
logp	2.858		Crippen Method
mcvol	151.200	ml/mol	McGowan Method
pc	2673.54	kPa	Joback Method
tb	510.44	K	Cheméo Relay (1.0)
tf	307.01	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	326.44	J/mol×K	565.04	Joback Method
cpg	381.80	J/mol×K	760.72	Joback Method
cpg	373.86	J/mol×K	728.11	Joback Method
cpg	365.43	J/mol×K	695.49	Joback Method
cpg	356.49	J/mol×K	662.88	Joback Method
cpg	347.03	J/mol×K	630.27	Joback Method
cpg	337.02	J/mol×K	597.65	Joback Method

dvisc	0.0007662	Pa×s	452.33	Joback Method
dvisc	0.0003317	Pa×s	565.04	Joback Method
dvisc	0.0004214	Pa×s	527.47	Joback Method
dvisc	0.0005553	Pa×s	489.90	Joback Method
dvisc	0.0030858	Pa×s	339.62	Joback Method
dvisc	0.0011207	Pa×s	414.76	Joback Method
dvisc	0.0017682	Pa×s	377.19	Joback Method

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=C10027073&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

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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
tf:	Normal melting (fusion) point

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