Fumaryl chloride

Other names:	Fumaroyl chloride
	2-Butenedioyl dichloride, (E)-
	Chlorure de fumaryle
	Dichlorid kyseliny fumarove
	Fumaroyl dichloride
	Fumarylchlorid
	TL 189
	UN 1780
	(2E)-2-Butenedioyl dichloride
	2-Butenedioyl dichloride, (2E)-
	Fumaryl dichloride
Inchi:	InChI=1S/C4H2Cl2O2/c5-3(7)1-2-4(6)8/h1-2H/b2-1+
InchiKey:	ZLYYJUJDFKGVKB-OWOJBTEDSA-N
Formula:	C4H2Cl2O2
SMILES:	O=C(Cl)C=CC(=O)Cl
Mol. weight [g/mol]:	152.96
CAS:	627-63-4

Physical Properties

Property code	Value	Unit	Source
gf	-218.68	kJ/mol	Joback Method
hf	-265.31	kJ/mol	Joback Method
hfus	17.91	kJ/mol	Joback Method
hvap	46.72	kJ/mol	Joback Method
log10ws	-1.21		Crippen Method
logp	1.073		Crippen Method
mcvol	90.540	ml/mol	McGowan Method
pc	4456.32	kPa	Joback Method
tb	432.20	K	NIST Webbook
tb	435.70	K	NIST Webbook
tc	694.89	K	Joback Method
tf	289.46	K	Joback Method
vc	0.349	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	169.11	J/mol×K	694.89	Joback Method
cpg	143.21	J/mol×K	477.68	Joback Method
cpg	148.44	J/mol×K	513.88	Joback Method
cpg	153.28	J/mol×K	550.08	Joback Method
cpg	157.74	J/mol×K	586.28	Joback Method
cpg	161.85	J/mol×K	622.48	Joback Method
cpg	165.63	J/mol×K	658.68	Joback Method
dvisc	0.0003909	Pa×s	477.68	Joback Method
dvisc	0.0030050	Pa×s	289.46	Joback Method
dvisc	0.0018115	Pa×s	320.83	Joback Method
dvisc	0.0011951	Pa×s	352.20	Joback Method
dvisc	0.0008439	Pa×s	383.57	Joback Method
dvisc	0.0006281	Pa×s	414.94	Joback Method
dvisc	0.0004873	Pa×s	446.31	Joback Method
hvapt	45.60	kJ/mol	360.50	NIST Webbook

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=C627634&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
hvapt: Enthalpy of vaporization at a given temperature

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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume