1,4-Benzenedicarbonyl dichloride

Other names:	1,4-Benzenedicarbonyl chloride
	NSC 41885
	Terephthalic acid chloride
	Terephthalic acid dichloride
	Terephthalic dichloride
	Terephthaloyl chloride
	Terephthaloyl dichloride
	Terephthalyl dichloride
	p-Phenylenedicarbonyl dichloride
	p-Phthaloyl chloride
	p-Phthaloyl dichloride
	p-Phthalyl dichloride
Inchi:	InChI=1S/C8H4Cl2O2/c9-7(11)5-1-2-6(4-3-5)8(10)12/h1-4H
InchiKey:	LXEJRKJRKIFVNY-UHFFFAOYSA-N
Formula:	C8H4Cl2O2
SMILES:	O=C(Cl)c1ccc(C(=O)Cl)cc1
Mol. weight [g/mol]:	203.02
CAS:	100-20-9

Physical Properties

Property code	Value	Unit	Source
chs	-3382.00 ± 3.00	kJ/mol	NIST Webbook
chs	-3380.80 ± 2.50	kJ/mol	NIST Webbook
gf	-162.44	kJ/mol	Joback Method
hf	-240.03	kJ/mol	Joback Method
hfs	-384.00	kJ/mol	NIST Webbook
hfs	-338.90 ± 2.50	kJ/mol	NIST Webbook
hfus	21.72	kJ/mol	Joback Method
hvap	58.60	kJ/mol	Joback Method
log10ws	-3.25		Crippen Method
logp	2.445		Crippen Method
mcvol	127.440	ml/mol	McGowan Method
pc	3819.82	kPa	Joback Method
ss	226.10	J/mol×K	NIST Webbook
tb	539.20	K	NIST Webbook
tc	838.34	K	Joback Method
tf	378.56	K	Joback Method

vc	0.485	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	255.95	J/mol×K	636.97	Joback Method
cpg	288.72	J/mol×K	838.34	Joback Method
cpg	283.38	J/mol×K	798.06	Joback Method
cpg	277.47	J/mol×K	757.79	Joback Method
cpg	270.94	J/mol×K	717.52	Joback Method
cpg	263.78	J/mol×K	677.25	Joback Method
cpg	247.41	J/mol×K	596.70	Joback Method
cps	207.90	J/mol×K	300.00	NIST Webbook
dvisc	0.0012716	Pa×s	414.92	Joback Method
dvisc	0.0008826	Pa×s	451.27	Joback Method
dvisc	0.0006468	Pa×s	487.63	Joback Method
dvisc	0.0004949	Pa×s	523.99	Joback Method
dvisc	0.0003921	Pa×s	560.34	Joback Method
dvisc	0.0019653	Pa×s	378.56	Joback Method
dvisc	0.0003196	Pa×s	596.70	Joback Method
hfust	21.10	kJ/mol	356.10	NIST Webbook
hfust	2.34	kJ/mol	337.30	NIST Webbook
hfust	21.10	kJ/mol	356.10	NIST Webbook
hvapt	56.20	kJ/mol	463.50	NIST Webbook
sfust	59.25	J/mol×K	356.10	NIST Webbook
sfust	6.92	J/mol×K	337.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.34936e+01
Coeff. B	-5.01164e+03
Temperature range (K), min.	379.50
Temperature range (K), max.	612.51

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C100209&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
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
pvap:	Vapor pressure
sfust:	Entropy of fusion at a given temperature
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume