Benzene, 1,4-bis(chloromethyl)-

Other names:	1,4-Bis(chloromethyl)benzene Benzene, p-bis(chloromethyl)- Dichlorodi-p-xylylene NSC 36976 alpha,alpha'-Dichloro-p-xylene p-Bis(chloromethyl)benzene p-Dichloroxylylene p-Xylene, «alpha»,«alpha»'-dichloro- p-Xylene, Â«alphaÂ»,Â«alphaÂ»'-dichloro- p-Xylene-«alpha»,«alpha»'-dichloride p-Xylene-Â«alphaÂ»,Â«alphaÂ»'-dichloride p-Xylylene chloride p-Xylylene dichloride «alpha»,«alpha»'-Dichloro-p-xylene Â«alphaÂ»,Â«alphaÂ»'-Dichloro-p-xylene
Inchi:	InChI=1S/C8H8Cl2/c9-5-7-1-2-8(6-10)4-3-7/h1-4H,5-6H2
InchiKey:	ZZHIDJWUJRKHGX-UHFFFAOYSA-N
Formula:	C8H8Cl2
SMILES:	ClCc1ccc(CCl)cc1
Mol. weight [g/mol]:	175.06
CAS:	623-25-6

Physical Properties

Property code	Value	Unit	Source
gf	95.40	kJ/mol	Joback Method
hf	-14.87	kJ/mol	Joback Method
hfus	18.52	kJ/mol	Joback Method
hvap	45.11	kJ/mol	Joback Method
log10ws	-3.54		Crippen Method
logp	3.164		Crippen Method
mcvol	124.300	ml/mol	McGowan Method
pc	3287.81	kPa	Joback Method
tb	527.20	K	NIST Webbook
tb	515.50 ± 2.50	K	NIST Webbook
tc	713.24	K	Joback Method
tf	341.40 ± 0.02	K	NIST Webbook
tf	373.00 ± 1.00	K	NIST Webbook

vc	0.473	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	282.97	J/mol×K	713.24	Joback Method
cpg	226.69	J/mol×K	488.96	Joback Method
cpg	237.74	J/mol×K	526.34	Joback Method
cpg	248.08	J/mol×K	563.72	Joback Method
cpg	257.74	J/mol×K	601.10	Joback Method
cpg	266.75	J/mol×K	638.48	Joback Method
cpg	275.15	J/mol×K	675.86	Joback Method
dvisc	0.0002727	Pa×s	488.96	Joback Method
dvisc	0.0023233	Pa×s	278.70	Joback Method
dvisc	0.0013318	Pa×s	313.74	Joback Method
dvisc	0.0008537	Pa×s	348.79	Joback Method
dvisc	0.0005936	Pa×s	383.83	Joback Method
dvisc	0.0004386	Pa×s	418.87	Joback Method
dvisc	0.0003395	Pa×s	453.92	Joback Method
hfust	23.97	kJ/mol	373.20	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	408.00	K	1.60	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.58921e+01
Coeff. B	-4.67695e+03
Coeff. C	-8.70030e+01
Temperature range (K), min.	386.72

Temperature range (K), max.	529.03

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C623256&Units=SI

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
hfust:	Enthalpy of fusion at a given temperature
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
pvap:	Vapor 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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