Benzene, 1,3-bis(chloromethyl)-

Other names:	1,3-Bis(chloromethyl)benzene m-Bis(chloromethyl)benzene m-Dichloroxylene m-Xylene, «alpha»,«alpha»'-dichloro- m-Xylene, Â«alphaÂ»,Â«alphaÂ»'-dichloro- m-Xylylene dichloride «alpha»,«alpha»'-Dichloro-m-xylene Â«alphaÂ»,Â«alphaÂ»'-Dichloro-m-xylene
Inchi:	InChI=1S/C8H8Cl2/c9-5-7-2-1-3-8(4-7)6-10/h1-4H,5-6H2
InchiKey:	GRJWOKACBGZOKT-UHFFFAOYSA-N
Formula:	C8H8Cl2
SMILES:	ClCc1cccc(CCl)c1
Mol. weight [g/mol]:	175.06
CAS:	626-16-4

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	525.70	K	NIST Webbook
tb	527.00	K	NIST Webbook
tc	713.24	K	Joback Method
tf	306.00 ± 1.00	K	NIST Webbook
tf	310.00 ± 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	275.15	J/mol×K	675.86	Joback Method
cpg	266.75	J/mol×K	638.48	Joback Method
cpg	257.74	J/mol×K	601.10	Joback Method
cpg	248.08	J/mol×K	563.72	Joback Method
cpg	237.74	J/mol×K	526.34	Joback Method
cpg	226.69	J/mol×K	488.96	Joback Method
dvisc	0.0023233	Pa×s	278.70	Joback Method
dvisc	0.0002727	Pa×s	488.96	Joback Method
dvisc	0.0003395	Pa×s	453.92	Joback Method
dvisc	0.0004386	Pa×s	418.87	Joback Method
dvisc	0.0005936	Pa×s	383.83	Joback Method
dvisc	0.0008537	Pa×s	348.79	Joback Method
dvisc	0.0013318	Pa×s	313.74	Joback Method
hfust	19.51	kJ/mol	307.20	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.40071e+01
Coeff. B	-4.11884e+03
Coeff. C	-8.70030e+01
Temperature range (K), min.	387.22
Temperature range (K), max.	560.67

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=C626164&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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

https://www.chemeo.com/cid/38-806-5/Benzene-1-3-bis-chloromethyl.pdf

Generated by Cheméo on 2024-10-12 04:22:52.552176869 +0000 UTC m=+3287835.189146120.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.