

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, Å«alphaÅ», Å«alphaÅ»'-dichloro- m-Xylylene dichloride «alpha», «alpha»'-Dichloro-m-xylene Å«alphaÅ», Å«alphaÅ»'-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:	ClC1cccc(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	527.00	K	NIST Webbook
tb	525.70	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	Paxs	278.70	Joback Method
dvisc	0.0002727	Paxs	488.96	Joback Method
dvisc	0.0003395	Paxs	453.92	Joback Method
dvisc	0.0004386	Paxs	418.87	Joback Method
dvisc	0.0005936	Paxs	383.83	Joback Method
dvisc	0.0008537	Paxs	348.79	Joback Method
dvisc	0.0013318	Paxs	313.74	Joback Method
hfust	19.51	kJ/mol	307.20	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
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

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
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/ci9903071

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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	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

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