

Benzene, 1,3-bis-(chloromethyl)-5-methyl

Inchi:	InChI=1S/C9H10Cl2/c1-7-2-8(5-10)4-9(3-7)6-11/h2-4H,5-6H2,1H3
InchiKey:	LGXPFAXLKHUJX-UHFFFAOYSA-N
Formula:	C9H10Cl2
SMILES:	Cc1cc(CCl)cc(CCl)c1
Mol. weight [g/mol]:	189.08

Physical Properties

Property code	Value	Unit	Source
gf	94.19	kJ/mol	Joback Method
hf	-46.98	kJ/mol	Joback Method
hfus	20.72	kJ/mol	Joback Method
hvap	48.00	kJ/mol	Joback Method
log10ws	-4.01		Crippen Method
logp	3.473		Crippen Method
mcvol	138.390	ml/mol	McGowan Method
pc	2906.11	kPa	Joback Method
rinpola	1402.00		NIST Webbook
tb	516.82	K	Joback Method
tc	738.55	K	Joback Method
tf	302.49	K	Joback Method
vc	0.529	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	268.32	J/molxK	516.82	Joback Method
cpg	320.64	J/molxK	701.60	Joback Method
cpg	311.46	J/molxK	664.64	Joback Method
cpg	301.67	J/molxK	627.69	Joback Method
cpg	291.23	J/molxK	590.73	Joback Method
cpg	280.12	J/molxK	553.78	Joback Method
cpg	329.23	J/molxK	738.55	Joback Method
dvisc	0.0002472	Paxs	516.82	Joback Method
dvisc	0.0003037	Paxs	481.10	Joback Method

dvisc	0.0003855	Paxs	445.38	Joback Method
dvisc	0.0005103	Paxs	409.66	Joback Method
dvisc	0.0007125	Paxs	373.93	Joback Method
dvisc	0.0010674	Paxs	338.21	Joback Method
dvisc	0.0017596	Paxs	302.49	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R131714&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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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