

1-Methyl-4-(1-methylethyl)-2,3-bis(chloromethyl)benzene

Inchi:	InChI=1S/C12H16Cl2/c1-8(2)10-5-4-9(3)11(6-13)12(10)7-14/h4-5,8H,6-7H2,1-3H3
InchiKey:	MBKXFZDCNSTKSD-UHFFFAOYSA-N
Formula:	C12H16Cl2
SMILES:	Cc1ccc(C(C)C)c(CCl)c1CCl
Mol. weight [g/mol]:	231.16

Physical Properties

Property code	Value	Unit	Source
gf	107.38	kJ/mol	Joback Method
hf	-125.65	kJ/mol	Joback Method
hfus	24.58	kJ/mol	Joback Method
hvap	54.95	kJ/mol	Joback Method
log10ws	-5.20		Crippen Method
logp	4.596		Crippen Method
mvol	180.660	ml/mol	McGowan Method
pc	2163.33	kPa	Joback Method
rinpol	1670.00		NIST Webbook
rinpol	1670.00		NIST Webbook
tb	590.00	K	Joback Method
tc	806.13	K	Joback Method
tf	333.82	K	Joback Method
vc	0.692	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	404.98	J/molxK	590.00	Joback Method
cpg	470.03	J/molxK	770.11	Joback Method
cpg	458.54	J/molxK	734.09	Joback Method
cpg	446.32	J/molxK	698.06	Joback Method
cpg	433.34	J/molxK	662.04	Joback Method
cpg	419.57	J/molxK	626.02	Joback Method
cpg	480.80	J/molxK	806.13	Joback Method
dvisc	0.0001789	Paxs	590.00	Joback Method

dvisc	0.0002240	Paxs	547.30	Joback Method
dvisc	0.0002913	Paxs	504.61	Joback Method
dvisc	0.0003978	Paxs	461.91	Joback Method
dvisc	0.0005788	Paxs	419.21	Joback Method
dvisc	0.0009168	Paxs	376.52	Joback Method
dvisc	0.0016337	Paxs	333.82	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=R520377&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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