

1,3,5-Trimethyl-2-(1-methylethyl)-4,6-bis(chloromethyl)benzene

Inchi:	InChI=1S/C14H20Cl2/c1-8(2)14-10(4)12(6-15)9(3)13(7-16)11(14)5/h8H,6-7H2,1-5H3
InchiKey:	UMPICIIHABYNKI-UHFFFAOYSA-N
Formula:	C14H20Cl2
SMILES:	Cc1c(CCl)c(C)c(C(C)C)c(C)c1CCl
Mol. weight [g/mol]:	259.21

Physical Properties

Property code	Value	Unit	Source
gf	104.96	kJ/mol	Joback Method
hf	-189.87	kJ/mol	Joback Method
hfus	28.98	kJ/mol	Joback Method
hvap	60.73	kJ/mol	Joback Method
log10ws	-6.15		Crippen Method
logp	5.213		Crippen Method
mcvol	208.840	ml/mol	McGowan Method
pc	1777.34	kPa	Joback Method
rinpol	1966.00		NIST Webbook
rinpol	1966.00		NIST Webbook
tb	645.72	K	Joback Method
tc	856.61	K	Joback Method
tf	381.40	K	Joback Method
vc	0.803	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	503.40	J/molxK	645.72	Joback Method
cpg	518.89	J/molxK	680.87	Joback Method
cpg	533.57	J/molxK	716.02	Joback Method
cpg	547.46	J/molxK	751.17	Joback Method
cpg	560.59	J/molxK	786.32	Joback Method
cpg	572.97	J/molxK	821.46	Joback Method
cpg	584.61	J/molxK	856.61	Joback Method
dvisc	0.0009850	Paxs	381.40	Joback Method

dvisc	0.0006065	Paxs	425.45	Joback Method
dvisc	0.0004090	Paxs	469.51	Joback Method
dvisc	0.0002951	Paxs	513.56	Joback Method
dvisc	0.0002242	Paxs	557.61	Joback Method
dvisc	0.0001773	Paxs	601.67	Joback Method
dvisc	0.0001448	Paxs	645.72	Joback Method

Sources

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=R520248&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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

Latest version available from:

<https://www.chemeo.com/cid/11-202-4/1-3-5-Trimethyl-2-1-methylethyl-4-6-bis-chloromethyl-benzene.pdf>

Generated by Cheméo on 2024-04-26 07:37:52.361822811 +0000 UTC m=+16406321.282400127.

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