Benzene, 1,4-bis(chloromethyl)-2,3,5,6-tetramethyl-

Other names: 3,6-Bis(chloromethyl)durene
Bis(chloromethyl)durene
1,2,4,5-Tetramethyl-3,6-bis(chloromethyl)benzene
1,4-Bis(chloromethyl)-2,3,5,6-tetramethylbenzene
1,4-Bis(chloromethyl)durene
2,3,5,6-Tetramethyl-p-dichloroxylene
1,4-Bis(chloromethyl)tetramethylbenzene
2,3,5,6-Tetramethyl-p-xylylene dichloride
2,3,5,6-Tetramethyl-p-dichloroxylylene
NSC 93952

Inchi: InChI=1S/C12H16Cl2/c1-7-8(2)12(6-14)10(4)9(3)11(7)5-13/h5-6H2,1-4H3

InchiKey: PGFAKOSRZYDFLR-UHFFFAOYSA-N

Formula: C12H16Cl2

SMILES: Cc1c(C)c(CCl)c(C)c(C)c1CCl

Mol. weight [g/mol]: 231.16

CAS: 3022-16-0

Physical Properties

Property code	Value	Unit	Source
gf	90.56	kJ/mol	Joback Method
hf	-143.31	kJ/mol	Joback Method
hfus	27.33	kJ/mol	Joback Method
hvap	56.66	kJ/mol	Joback Method
log10ws	-5.44		Crippen Method
logp	4.398		Crippen Method
mcvol	180.660	ml/mol	McGowan Method
pc	2088.84	kPa	Joback Method
rinpol	1867.00		NIST Webbook
rinpol	1867.00		NIST Webbook
tb	600.40	K	Joback Method
tc	814.03	K	Joback Method
tf	373.86	K	Joback Method
vc	0.698	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	403.40	J/mol×K	600.40	Joback Method
cpg	417.17	J/mol×K	636.01	Joback Method
cpg	430.26	J/mol×K	671.61	Joback Method
cpg	442.69	J/mol×K	707.22	Joback Method
cpg	454.45	J/mol×K	742.82	Joback Method
cpg	465.58	J/mol×K	778.43	Joback Method
cpg	476.07	J/mol×K	814.03	Joback Method
dvisc	0.0008975	Pa×s	373.86	Joback Method
dvisc	0.0006121	Pa×s	411.62	Joback Method
dvisc	0.0004452	Pa×s	449.37	Joback Method
dvisc	0.0003401	Pa×s	487.13	Joback Method
dvisc	0.0002701	Pa×s	524.89	Joback Method
dvisc	0.0002213	Pa×s	562.64	Joback Method
dvisc	0.0001859	Pa×s	600.40	Joback Method

Sources

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=C3022160&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