1-Methyl-4-(1-methylethyl)-2,6-bis(chloromethyl)b

Inchi: InChI=1S/C12H16Cl2/c1-8(2)10-4-11(6-13)9(3)12(5-10)7-14/h4-5,8H,6-7H2,1-3H3
InchiKey: ATKWAVDYPVPWEH-UHFFFAOYSA-N
Formula: C12H16Cl2
SMILES: Cc1c(CCl)cc(C(C)C)cc1CCl
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
mcvol	180.660	ml/mol	McGowan Method
pc	2163.33	kPa	Joback Method
rinpol	1709.00		NIST Webbook
rinpol	1709.00		NIST Webbook
tb	590.00	K	Joback Method
tc	806.13	K	Joback Method
tf	333.82	K	Joback Method
vc	0.692	m3/kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0002240	Pa×s	547.30	Joback Method
dvisc	0.0002913	Pa×s	504.61	Joback Method
dvisc	0.0003978	Pa×s	461.91	Joback Method
dvisc	0.0005788	Pa×s	419.21	Joback Method
dvisc	0.0009168	Pa×s	376.52	Joback Method
dvisc	0.0016337	Pa×s	333.82	Joback Method

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=R520397&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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