1-Chloromethyl-3,5-bis(1,1-dimethylethyl)benzene

Other names: Benzene,1-(chloromethyl)-3,5-bis(1,1-dimethylethyl)-
Inchi: InChI=1S/C15H23Cl/c1-14(2,3)12-7-11(10-16)8-13(9-12)15(4,5)6/h7-9H,10H2,1-6H3
InchiKey: UNRGFCVSCXJGCL-UHFFFAOYSA-N
Formula: C15H23Cl
SMILES: CC(C)(C)c1cc(CCl)cc(C(C)(C)C)c1
Mol. weight [g/mol]: 238.80
CAS: 51625-14-0

Physical Properties

Property code	Value	Unit	Source
gf	162.32	kJ/mol	Joback Method
hf	-172.58	kJ/mol	Joback Method
hfus	17.24	kJ/mol	Joback Method
hvap	54.38	kJ/mol	Joback Method
ie	8.29 ± 0.03	eV	NIST Webbook
log10ws	-5.13		Crippen Method
logp	5.020		Crippen Method
mcvol	210.690	ml/mol	McGowan Method
pc	1801.56	kPa	Joback Method
tb	610.21	K	Joback Method
tc	831.24	K	Joback Method
tf	345.03	K	Joback Method
vc	0.794	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	531.75	J/mol×K	610.21	Joback Method
cpg	550.76	J/mol×K	647.05	Joback Method
cpg	568.46	J/mol×K	683.89	Joback Method
cpg	584.95	J/mol×K	720.73	Joback Method
cpg	600.32	J/mol×K	757.57	Joback Method
cpg	614.66	J/mol×K	794.41	Joback Method
cpg	628.05	J/mol×K	831.24	Joback Method

dvisc	0.0021864	Pa×s	345.03	Joback Method
dvisc	0.0010236	Pa×s	389.23	Joback Method
dvisc	0.0005594	Pa×s	433.42	Joback Method
dvisc	0.0003419	Pa×s	477.62	Joback Method
dvisc	0.0002271	Pa×s	521.82	Joback Method
dvisc	0.0001609	Pa×s	566.01	Joback Method
dvisc	0.0001197	Pa×s	610.21	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=C51625140&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume