Benzene, 1,3,5-tris(chloromethyl)-2,4,6-trimethyl-

Other names: 1,3,5-Trimethyl-2,4,6-tris(chloromethyl)benzene
Inchi: InChI=1S/C12H15Cl3/c1-7-10(4-13)8(2)12(6-15)9(3)11(7)5-14/h4-6H2,1-3H3
InchiKey: PHQFMPNZCIHSPC-UHFFFAOYSA-N
Formula: C12H15Cl3
SMILES: Cc1c(CCl)c(C)c(CCl)c(C)c1CCl
Mol. weight [g/mol]: 265.61
CAS: 3849-01-2

Physical Properties

Property code	Value	Unit	Source
gf	78.63	kJ/mol	Joback Method
hf	-159.05	kJ/mol	Joback Method
hfus	31.52	kJ/mol	Joback Method
hvap	61.05	kJ/mol	Joback Method
log10ws	-6.00		Crippen Method
logp	4.828		Crippen Method
mcvol	192.900	ml/mol	McGowan Method
pc	2019.95	kPa	Joback Method
rinpol	2073.00		NIST Webbook
rinpol	2073.00		NIST Webbook
tb	637.83	K	Joback Method
tc	855.06	K	Joback Method
tf	403.78	K	Joback Method
vc	0.747	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	429.11	J/mol×K	637.83	Joback Method
cpg	442.08	J/mol×K	674.04	Joback Method
cpg	454.35	J/mol×K	710.24	Joback Method
cpg	465.94	J/mol×K	746.45	Joback Method
cpg	476.87	J/mol×K	782.65	Joback Method
cpg	487.15	J/mol×K	818.86	Joback Method

cpg	496.81	J/mol×K	855.06	Joback Method
dvisc	0.0008623	Pa×s	403.78	Joback Method
dvisc	0.0005910	Pa×s	442.79	Joback Method
dvisc	0.0004306	Pa×s	481.80	Joback Method
dvisc	0.0003290	Pa×s	520.81	Joback Method
dvisc	0.0002610	Pa×s	559.81	Joback Method
dvisc	0.0002134	Pa×s	598.82	Joback Method
dvisc	0.0001788	Pa×s	637.83	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=C3849012&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

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