1-Phenyl-3-chloro-2,2-bis(chloromethyl)-1-propan

Inchi: InChI=1S/C11H11Cl3O/c12-6-11(7-13,8-14)10(15)9-4-2-1-3-5-9/h1-5H,6-8H2
InchiKey: VOGMUJBKJVSTGJ-UHFFFAOYSA-N
Formula: C11H11Cl3O
SMILES: O=C(c1ccccc1)C(CCl)(CCl)CCl
Mol. weight [g/mol]: 265.56

Physical Properties

Property code	Value	Unit	Source
gf	-7.72	kJ/mol	Joback Method
hf	-202.39	kJ/mol	Joback Method
hfus	25.06	kJ/mol	Joback Method
hvap	60.96	kJ/mol	Joback Method
log10ws	-3.61		Crippen Method
logp	3.572		Crippen Method
mcvol	180.380	ml/mol	McGowan Method
pc	2571.50	kPa	Joback Method
rinpol	1814.00		NIST Webbook
tb	640.69	K	Joback Method
tc	877.42	K	Joback Method
tf	382.26	K	Joback Method
vc	0.685	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	402.86	J/mol×K	640.69	Joback Method
cpg	415.19	J/mol×K	680.15	Joback Method
cpg	426.46	J/mol×K	719.60	Joback Method
cpg	436.76	J/mol×K	759.06	Joback Method
cpg	446.17	J/mol×K	798.51	Joback Method
cpg	454.78	J/mol×K	837.97	Joback Method
cpg	462.68	J/mol×K	877.42	Joback Method
dvisc	0.0023038	Pa×s	382.26	Joback Method
dvisc	0.0012263	Pa×s	425.33	Joback Method

dvisc	0.0007330	Pa×s	468.40	Joback Method
dvisc	0.0004778	Pa×s	511.48	Joback Method
dvisc	0.0003329	Pa×s	554.55	Joback Method
dvisc	0.0002443	Pa×s	597.62	Joback Method
dvisc	0.0001869	Pa×s	640.69	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=R520491&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