1-Phenyl-2,2-bis(chloromethyl)-1-butanone

Inchi: InChI=1S/C12H14Cl2O/c1-2-12(8-13,9-14)11(15)10-6-4-3-5-7-10/h3-7H,2,8-9H2,1H3
InchiKey: ADOXRJBMXKQBCH-UHFFFAOYSA-N
Formula: C12H14Cl2O
SMILES: CCC(CCl)(CCl)C(=O)c1ccccc1
Mol. weight [g/mol]: 245.15

Physical Properties

Property code	Value	Unit	Source
gf	12.63	kJ/mol	Joback Method
hf	-207.29	kJ/mol	Joback Method
hfus	23.46	kJ/mol	Joback Method
hvap	58.80	kJ/mol	Joback Method
log10ws	-3.87		Crippen Method
logp	3.743		Crippen Method
mcvol	182.230	ml/mol	McGowan Method
pc	2424.27	kPa	Joback Method
rinpol	1705.00		NIST Webbook
tb	626.14	K	Joback Method
tc	855.03	K	Joback Method
tf	363.61	K	Joback Method
vc	0.693	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	426.85	J/mol×K	626.14	Joback Method
cpg	441.02	J/mol×K	664.29	Joback Method
cpg	454.08	J/mol×K	702.44	Joback Method
cpg	466.12	J/mol×K	740.59	Joback Method
cpg	477.21	J/mol×K	778.73	Joback Method
cpg	487.43	J/mol×K	816.88	Joback Method
cpg	496.87	J/mol×K	855.03	Joback Method
dvisc	0.0026032	Pa×s	363.61	Joback Method
dvisc	0.0013184	Pa×s	407.37	Joback Method

dvisc	0.0007619	Pa×s	451.12	Joback Method
dvisc	0.0004851	Pa×s	494.88	Joback Method
dvisc	0.0003324	Pa×s	538.63	Joback Method
dvisc	0.0002411	Pa×s	582.38	Joback Method
dvisc	0.0001829	Pa×s	626.14	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R520446&Units=SI
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

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