Cyclopropane, 1,1-dichloro-2-(4-phenylbutyl)

Inchi: InChI=1S/C13H16Cl2/c14-13(15)10-12(13)9-5-4-8-11-6-2-1-3-7-11/h1-3,6-7,12H,4-5,8-1
InchiKey: FDUMPPULNMGIOO-UHFFFAOYSA-N
Formula: C13H16Cl2
SMILES: ClC1(Cl)CC1CCCCc1ccccc1
Mol. weight [g/mol]: 243.17

Physical Properties

Property code	Value	Unit	Source
gf	194.68	kJ/mol	Joback Method
hf	-38.90	kJ/mol	Joback Method
hfus	24.77	kJ/mol	Joback Method
hvap	54.03	kJ/mol	Joback Method
log10ws	-4.93		Crippen Method
logp	4.593		Crippen Method
mcvol	183.890	ml/mol	McGowan Method
pc	2340.56	kPa	Joback Method
rinpol	1685.00		NIST Webbook
rinpol	1685.00		NIST Webbook
ripol	2191.00		NIST Webbook
ripol	2191.00		NIST Webbook
tb	600.69	K	Joback Method
tc	829.37	K	Joback Method
tf	360.13	K	Joback Method
vc	0.708	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	439.95	J/mol×K	600.69	Joback Method
cpg	456.34	J/mol×K	638.80	Joback Method
cpg	471.61	J/mol×K	676.92	Joback Method
cpg	485.93	J/mol×K	715.03	Joback Method
cpg	499.50	J/mol×K	753.15	Joback Method
cpg	512.51	J/mol×K	791.26	Joback Method

cpg	525.12	J/mol×K	829.37	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R122022&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

Legend

cpg:	Ideal gas heat capacity
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume