Cyclopropane, 1,1-dichloro-2-butyl-3-phenyl

Inchi: InChI=1S/C13H16Cl2/c1-2-3-9-11-12(13(11,14)15)10-7-5-4-6-8-10/h4-8,11-12H,2-3,9H2
InchiKey: QGEAMIYGNOJAQK-UHFFFAOYSA-N
Formula: C13H16Cl2
SMILES: CCCCC1C(c2ccccc2)C1(Cl)Cl
Mol. weight [g/mol]: 243.17

Physical Properties

Property code	Value	Unit	Source
gf	186.97	kJ/mol	Joback Method
hf	-59.24	kJ/mol	Joback Method
hfus	25.84	kJ/mol	Joback Method
hvap	53.72	kJ/mol	Joback Method
log10ws	-4.90		Crippen Method
logp	4.764		Crippen Method
mcvol	183.890	ml/mol	McGowan Method
pc	2267.57	kPa	Joback Method
rinpol	1596.00		NIST Webbook
rinpol	1596.00		NIST Webbook
ripol	2075.00		NIST Webbook
ripol	2075.00		NIST Webbook
tb	596.02	K	Joback Method
tc	824.74	K	Joback Method
tf	355.89	K	Joback Method
vc	0.707	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	441.72	J/mol×K	596.02	Joback Method
cpg	458.63	J/mol×K	634.14	Joback Method
cpg	474.40	J/mol×K	672.26	Joback Method
cpg	489.20	J/mol×K	710.38	Joback Method
cpg	503.21	J/mol×K	748.50	Joback Method
cpg	516.61	J/mol×K	786.62	Joback Method

cpg	529.56	J/mol×K	824.74	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R122037&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
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