Benzene, (cyclopentylidenephenylmethyl)-

Inchi: InChI=1S/C18H18/c1-3-9-15(10-4-1)18(17-13-7-8-14-17)16-11-5-2-6-12-16/h1-6,9-12H,7
InchiKey: POPQCIZUXRKKGP-UHFFFAOYSA-N
Formula: C18H18
SMILES: c1ccc(C(=C2CCCC2)c2ccccc2)cc1
Mol. weight [g/mol]: 234.34
CAS: 7714-72-9

Physical Properties

Property code	Value	Unit	Source
gf	406.67	kJ/mol	Joback Method
hf	205.27	kJ/mol	Joback Method
hfus	22.34	kJ/mol	Joback Method
hvap	61.65	kJ/mol	Joback Method
log10ws	-5.58		Crippen Method
logp	5.062		Crippen Method
mcvol	201.800	ml/mol	McGowan Method
pc	2410.00	kPa	Joback Method
tb	691.07	K	Joback Method
tc	955.53	K	Joback Method
tf	334.20 ± 2.00	K	NIST Webbook
tf	335.00 ± 4.00	K	NIST Webbook
vc	0.753	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	542.34	J/mol×K	691.07	Joback Method
cpg	562.65	J/mol×K	735.15	Joback Method
cpg	581.20	J/mol×K	779.22	Joback Method
cpg	598.14	J/mol×K	823.30	Joback Method
cpg	613.65	J/mol×K	867.38	Joback Method
cpg	627.88	J/mol×K	911.45	Joback Method
cpg	641.01	J/mol×K	955.53	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7714729&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume