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

Physical Properties

Property code	Value	Unit	Source
hfus	22.34	kJ/mol	Joback Method
ie	7.87	eV	Cheméo Relay (1.0)
logp	5.062		Crippen Method
mcvol	201.800	ml/mol	McGowan Method
tb	619.26	K	Cheméo Relay (1.0)
tf	335.00 ± 4.00	K	NIST Webbook
tf	334.20 ± 2.00	K	NIST Webbook

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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7714729&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point