

1,1'-Diphenyl-1,1'-bicyclooctyl

Inchi: InChI=1S/C28H38/c1-3-13-21-27(22-14-4-1,25-17-9-7-10-18-25)28(26-19-11-8-12-20-26)
InchiKey: SKPRQLZOAQUBAG-UHFFFAOYSA-N
Formula: C28H38
SMILES: c1ccc(C2(C3(c4cccc4)CCCCC3)CCCCC2)cc1
Mol. weight [g/mol]: 374.60
CAS: 59358-73-5

Physical Properties

Property code	Value	Unit	Source
chs	-16344.10 ± 2.30	kJ/mol	NIST Webbook
gf	399.22	kJ/mol	Joback Method
hf	69.00 ± 3.00	kJ/mol	NIST Webbook
hfs	-104.90 ± 2.30	kJ/mol	NIST Webbook
hfus	19.03	kJ/mol	Joback Method
hsub	174.00	kJ/mol	NIST Webbook
hsub	173.90	kJ/mol	NIST Webbook
hvap	81.72	kJ/mol	Joback Method
log10ws	-8.89		Crippen Method
logp	8.351		Crippen Method
mvol	336.140	ml/mol	McGowan Method
pc	1430.46	kPa	Joback Method
tb	950.06	K	Joback Method
tc	1238.91	K	Joback Method
tf	506.64	K	Joback Method
vc	1.218	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1320.39	J/mol×K	1142.62	Joback Method
cpg	1357.37	J/mol×K	1190.76	Joback Method
cpg	1183.96	J/mol×K	950.06	Joback Method
cpg	1217.50	J/mol×K	998.20	Joback Method
cpg	1251.03	J/mol×K	1046.34	Joback Method

cpg	1285.13	J/mol×K	1094.48	Joback Method
cpg	1396.68	J/mol×K	1238.91	Joback Method
cps	453.80	J/mol×K	298.00	NIST Webbook
hfust	35.98	kJ/mol	432.00	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C59358735&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation 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

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