

Dispiro[cyclopropane-1,2'-bicyclo[2.2.2]octane-3',1'-cyclopropane]

Other names:	Dispiro[cyclopropane-1,2'-bicyclo[2.2.2]octane-3',1'-cyclopropane]
Inchi:	InChI=1S/C12H18/c1-2-10-4-3-9(1)11(5-6-11)12(10)7-8-12/h9-10H,1-8H2
InchiKey:	OBJLCEPMWWZOLB-UHFFFAOYSA-N
Formula:	C12H18
SMILES:	C1CC2CCC1C1(CC1)C21CC1
Mol. weight [g/mol]:	162.27
CAS:	40827-30-3

Physical Properties

Property code	Value	Unit	Source
gf	282.18	kJ/mol	Joback Method
hf	30.67	kJ/mol	Joback Method
hfus	6.78	kJ/mol	Joback Method
hvap	39.66	kJ/mol	Joback Method
ie	8.67	eV	NIST Webbook
ie	8.30	eV	NIST Webbook
log10ws	-3.46		Crippen Method
logp	3.367		Crippen Method
mcvol	136.500	ml/mol	McGowan Method
pc	3228.31	kPa	Joback Method
tb	501.40	K	Joback Method
tc	737.21	K	Joback Method
tf	344.56	K	Joback Method
vc	0.531	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	354.32	J/mol×K	501.40	Joback Method
cpg	376.50	J/mol×K	540.70	Joback Method
cpg	396.36	J/mol×K	580.00	Joback Method
cpg	414.31	J/mol×K	619.31	Joback Method
cpg	430.77	J/mol×K	658.61	Joback Method
cpg	446.13	J/mol×K	697.91	Joback Method

Sources

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=C40827303&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	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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