Dispiro[2.0.2.2]octane

Inchi: InChI=1S/C8H12/c1-2-7(1)5-6-8(7)3-4-8/h1-6H2
InchiKey: KHCZAHBPHDGNJP-UHFFFAOYSA-N
Formula: C8H12
SMILES: C1CC12CCC21CC1
Mol. weight [g/mol]: 108.18
CAS: 21426-37-9

Physical Properties

Property code	Value	Unit	Source
gf	207.56	kJ/mol	Joback Method
hf	66.93	kJ/mol	Joback Method
hfus	-0.69	kJ/mol	Joback Method
hvap	30.98	kJ/mol	Joback Method
ie	9.02	eV	NIST Webbook
ie	8.40	eV	NIST Webbook
log10ws	-2.37		Crippen Method
logp	2.341		Crippen Method
mcvol	91.000	ml/mol	McGowan Method
pc	4456.32	kPa	Joback Method
tb	403.54	K	Joback Method
tc	625.33	K	Joback Method
tf	289.30	K	Joback Method
vc	0.359	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	260.49	J/mol×K	588.36	Joback Method
cpg	188.62	J/mol×K	403.54	Joback Method
cpg	207.12	J/mol×K	440.50	Joback Method
cpg	223.24	J/mol×K	477.47	Joback Method
cpg	237.30	J/mol×K	514.43	Joback Method
cpg	249.61	J/mol×K	551.40	Joback Method
cpg	270.24	J/mol×K	625.33	Joback Method

hvapt	38.30	kJ/mol	324.50	NIST Webbook

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=C21426379&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
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
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