

Trispiro[2.0.2.0.2.0]nonane

Inchi:	InChI=1S/C9H12/c1-2-7(1)8(3-4-8)9(7)5-6-9/h1-6H2
InchiKey:	HAIZYAZVYQEJME-UHFFFAOYSA-N
Formula:	C9H12
SMILES:	C1CC12C1(CC1)C21CC1
Mol. weight [g/mol]:	120.19
CAS:	31561-59-8

Physical Properties

Property code	Value	Unit	Source
chl	-5638.10 ± 4.80	kJ/mol	NIST Webbook
gf	295.44	kJ/mol	Joback Method
hf	423.60 ± 4.90	kJ/mol	NIST Webbook
hfl	381.50 ± 4.90	kJ/mol	NIST Webbook
hfus	-2.06	kJ/mol	Joback Method
hvap	42.10	kJ/mol	NIST Webbook
ie	9.12	eV	NIST Webbook
log10ws	-2.44		Crippen Method
logp	2.341		Crippen Method
mcvol	94.230	ml/mol	McGowan Method
pc	4634.00	kPa	Joback Method
tb	424.86	K	Joback Method
tc	654.85	K	Joback Method
tf	349.45	K	Joback Method
vc	0.387	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	267.23	J/mol×K	539.86	Joback Method
cpg	278.55	J/mol×K	578.19	Joback Method
cpg	288.32	J/mol×K	616.52	Joback Method
cpg	218.86	J/mol×K	424.86	Joback Method
cpg	237.89	J/mol×K	463.19	Joback Method
cpg	253.85	J/mol×K	501.52	Joback Method

cpg	297.05	J/mol×K	654.85	Joback Method
hfust	14.14	kJ/mol	312.10	NIST Webbook
hvapt	59.20 ± 0.50	kJ/mol	290.50	NIST Webbook
hvapt	42.10 ± 0.60	kJ/mol	303.00	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=C31561598&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
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

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