

cis,trans-Cyclonona-1,5-diene

Inchi:	InChI=1S/C9H14/c1-2-4-6-8-9-7-5-3-1/h1-2,7,9H,3-6,8H2/b2-1-,9-7+
InchiKey:	UWMOLRCQDVCRLG-UYIJSCIWSA-N
Formula:	C9H14
SMILES:	C1=CCCCC=CCC1
Mol. weight [g/mol]:	122.21
CAS:	15753-74-9

Physical Properties

Property code	Value	Unit	Source
gf	80.68	kJ/mol	Joback Method
hf	-57.35	kJ/mol	Joback Method
hfus	5.97	kJ/mol	Joback Method
hvap	37.47	kJ/mol	Joback Method
log10ws	-3.19		Crippen Method
logp	3.063		Crippen Method
mvol	118.210	ml/mol	McGowan Method
pc	3472.45	kPa	Joback Method
tb	440.67	K	Joback Method
tc	670.68	K	Joback Method
tf	193.77	K	Joback Method
vc	0.421	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	224.76	J/molxK	440.67	Joback Method
cpg	309.64	J/molxK	632.35	Joback Method
cpg	294.72	J/molxK	594.01	Joback Method
cpg	278.79	J/molxK	555.68	Joback Method
cpg	261.83	J/molxK	517.34	Joback Method
cpg	243.83	J/molxK	479.01	Joback Method
cpg	323.56	J/molxK	670.68	Joback Method
dvisc	0.0001658	Paxs	440.67	Joback Method
dvisc	0.0002633	Paxs	399.52	Joback Method

dvisc	0.0004649	Paxs	358.37	Joback Method
dvisc	0.0009515	Paxs	317.22	Joback Method
dvisc	0.0024107	Paxs	276.07	Joback Method
dvisc	0.0084589	Paxs	234.92	Joback Method
dvisc	0.0505874	Paxs	193.77	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=C15753749&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
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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