

Tricyclo[4.2.0.0^{2,5}]octa-3,7-diene, (1«alpha»,2«alpha»,5«alpha»,6«alpha»)

Inchi:	InChI=1S/C8H8/c1-2-6-5(1)7-3-4-8(6)7/h1-8H/t5-,6+,7-,8+
InchiKey:	DUZZYQHCABHRAJ-KVFPUHGPSA-N
Formula:	C8H8
SMILES:	C1=CC2C1C1C=CC21
Mol. weight [g/mol]:	104.15
CAS:	20380-30-7

Physical Properties

Property code	Value	Unit	Source
gf	263.04	kJ/mol	Joback Method
hf	111.33	kJ/mol	Joback Method
hfus	16.50	kJ/mol	Joback Method
hvap	33.24	kJ/mol	Joback Method
ie	9.08	eV	NIST Webbook
ie	8.20 ± 0.10	eV	NIST Webbook
ie	9.08	eV	NIST Webbook
log10ws	-1.60		Crippen Method
logp	1.604		Crippen Method
mcvol	82.400	ml/mol	McGowan Method
pc	3995.65	kPa	Joback Method
tb	392.04	K	Joback Method
tc	597.54	K	Joback Method
tf	234.54	K	Joback Method
vc	0.334	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	162.04	J/mol×K	392.04	Joback Method
cpg	176.96	J/mol×K	426.29	Joback Method
cpg	190.62	J/mol×K	460.54	Joback Method
cpg	203.12	J/mol×K	494.79	Joback Method
cpg	214.54	J/mol×K	529.04	Joback Method
cpg	224.99	J/mol×K	563.29	Joback Method

cpg	234.57	J/molxK	597.54	Joback Method
dvisc	0.0001005	Paxs	234.54	Joback Method
dvisc	0.0001637	Paxs	260.79	Joback Method
dvisc	0.0002438	Paxs	287.04	Joback Method
dvisc	0.0003397	Paxs	313.29	Joback Method
dvisc	0.0004497	Paxs	339.54	Joback Method
dvisc	0.0005718	Paxs	365.79	Joback Method
dvisc	0.0007040	Paxs	392.04	Joback Method

Sources

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=C20380307&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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
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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