

Tricyclo[3.2.1.0^{2,4}]oct-6-ene,(1 «alpha»,2 «beta»,4 «gamma»)

Inchi:	InChI=1S/C8H10/c1-2-6-3-5(1)7-4-8(6)7/h1-2,5-8H,3-4H2/t5-,6-,7-,8+/m1/s1
InchiKey:	ZYVIMZRTFMWLDQ-XUTV FYLZSA-N
Formula:	C8H10
SMILES:	C1=CC2CC1C1CC21
Mol. weight [g/mol]:	106.17
CAS:	3635-95-8

Physical Properties

Property code	Value	Unit	Source
gf	233.08	kJ/mol	Joback Method
hf	231.00 ± 0.40	kJ/mol	NIST Webbook
hf	213.00 ± 4.20	kJ/mol	NIST Webbook
hfl	170.60 ± 1.40	kJ/mol	NIST Webbook
hfus	15.27	kJ/mol	Joback Method
hvap	42.40	kJ/mol	NIST Webbook
ie	8.90	eV	NIST Webbook
log10ws	-1.74		Crippen Method
logp	1.828		Crippen Method
mcvol	86.700	ml/mol	McGowan Method
pc	3819.82	kPa	Joback Method
tb	392.88	K	Joback Method
tc	596.21	K	Joback Method
tf	233.78	K	Joback Method
vc	0.347	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	174.43	J/mol×K	392.88	Joback Method
cpg	243.65	J/mol×K	562.32	Joback Method
cpg	231.99	J/mol×K	528.44	Joback Method
cpg	219.33	J/mol×K	494.55	Joback Method
cpg	205.57	J/mol×K	460.66	Joback Method
cpg	190.64	J/mol×K	426.77	Joback Method

cpg	254.40	J/molxK	596.21	Joback Method
dvisc	0.0007604	Paxs	392.88	Joback Method
dvisc	0.0006277	Paxs	366.36	Joback Method
dvisc	0.0005030	Paxs	339.85	Joback Method
dvisc	0.0003881	Paxs	313.33	Joback Method
dvisc	0.0002855	Paxs	286.81	Joback Method
dvisc	0.0001973	Paxs	260.30	Joback Method
dvisc	0.0001254	Paxs	233.78	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C3635958&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
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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