Tricyclo[4.2.0.02,5]octa-3,7-diene, (1«alpha»,2«beta»,5«beta»,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-SOSBWXJGSA-N

Formula: C8H8

SMILES: C1=CC2C1C1C=CC21

Mol. weight [g/mol]: 104.15

CAS: 20380-31-8

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	8.90	eV	NIST Webbook
ie	8.27 ± 0.10	eV	NIST Webbook
ie	8.96	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	m3/kmol	Joback Method

Temperature Dependent Properties

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

cpg	234.57	J/mol×K	597.54	Joback Method
dvisc	0.0007040	Pa×s	392.04	Joback Method
dvisc	0.0005718	Pa×s	365.79	Joback Method
dvisc	0.0004497	Pa×s	339.54	Joback Method
dvisc	0.0003397	Pa×s	313.29	Joback Method
dvisc	0.0002438	Pa×s	287.04	Joback Method
dvisc	0.0001637	Pa×s	260.79	Joback Method
dvisc	0.0001005	Pa×s	234.54	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C20380318&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
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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