Tricyclo[3.2.1.02,4]oct-6-ene,(1«alpha»,2«alpha»,4

Other names: Tricyclo[3,2,1,0(2,4)]oct-6-ene
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-XUTVFYLZSA-N
Formula: C8H10
SMILES: C1=CC2CC1C1CC21
Mol. weight [g/mol]: 106.17
CAS: 3635-94-7

Physical Properties

Property code	Value	Unit	Source
gf	233.08	kJ/mol	Joback Method
hf	239.00 ± 0.80	kJ/mol	NIST Webbook
hf	247.00 ± 4.20	kJ/mol	NIST Webbook
hfs	202.90 ± 1.30	kJ/mol	NIST Webbook
hfus	15.27	kJ/mol	Joback Method
hsub	44.10	kJ/mol	NIST Webbook
hvap	32.95	kJ/mol	Joback Method
ie	9.05	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	m3/kmol	Joback Method

Temperature Dependent Properties

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

cpg	231.99	J/mol×K	528.44	Joback Method
cpg	243.65	J/mol×K	562.32	Joback Method
cpg	254.40	J/mol×K	596.21	Joback Method
dvisc	0.0001254	Pa×s	233.78	Joback Method
dvisc	0.0001973	Pa×s	260.30	Joback Method
dvisc	0.0002855	Pa×s	286.81	Joback Method
dvisc	0.0003881	Pa×s	313.33	Joback Method
dvisc	0.0005030	Pa×s	339.85	Joback Method
dvisc	0.0006277	Pa×s	366.36	Joback Method
dvisc	0.0007604	Pa×s	392.88	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3635947&Units=SI
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

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfs: Solid phase enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hsub: Enthalpy of sublimation 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