trans-Cyclooctene

Other names: Cyclooctene, (E)-
Inchi: InChI=1S/C8H14/c1-2-4-6-8-7-5-3-1/h1-2H,3-8H2/b2-1+
InchiKey: URYYVOIYTNXXBN-OWOJBTEDSA-N
Formula: C8H14
SMILES: C1=CCCCCCC1
Mol. weight [g/mol]: 110.20
CAS: 931-89-5

Physical Properties

Property code	Value	Unit	Source
gf	54.40	kJ/mol	Joback Method
hf	20.00	kJ/mol	NIST Webbook
hf	19.60 ± 3.00	kJ/mol	NIST Webbook
hfus	4.26	kJ/mol	Joback Method
hvap	34.78	kJ/mol	Joback Method
log10ws	-2.92		Crippen Method
logp	2.897		Crippen Method
mcvol	108.420	ml/mol	McGowan Method
pc	3620.24	kPa	Joback Method
rinpol	899.00		NIST Webbook
rinpol	899.00		NIST Webbook
rinpol	899.00		NIST Webbook
tb	414.36	K	Joback Method
tc	635.63	K	Joback Method
tf	250.00 ± 10.00	K	NIST Webbook
tf	214.00 ± 5.00	K	NIST Webbook
vc	0.388	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	197.28	J/mol×K	414.36	Joback Method
cpg	215.41	J/mol×K	451.24	Joback Method
cpg	232.58	J/mol×K	488.12	Joback Method

cpg	248.81	J/mol×K	524.99	Joback Method
cpg	264.12	J/mol×K	561.87	Joback Method
cpg	278.54	J/mol×K	598.75	Joback Method
cpg	292.07	J/mol×K	635.63	Joback Method
dvisc	0.0426132	Pa×s	185.26	Joback Method
dvisc	0.0083526	Pa×s	223.44	Joback Method
dvisc	0.0026344	Pa×s	261.63	Joback Method
dvisc	0.0011148	Pa×s	299.81	Joback Method
dvisc	0.0005729	Pa×s	337.99	Joback Method
dvisc	0.0003370	Pa×s	376.18	Joback Method
dvisc	0.0002186	Pa×s	414.36	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C931895&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
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
mcvol: McGowan's characteristic volume
pc: Critical Pressure
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume