Ethylidenecycloheptane

Inchi: InChI=1S/C9H16/c1-2-9-7-5-3-4-6-8-9/h2H,3-8H2,1H3
InchiKey: MLFGNFYXTYMGAT-UHFFFAOYSA-N
Formula: C9H16
SMILES: CC=C1CCCCCC1
Mol. weight [g/mol]: 124.22
CAS: 10494-87-8

Physical Properties

Property code	Value	Unit	Source
gf	90.42	kJ/mol	Joback Method
hf	-84.56	kJ/mol	Joback Method
hfus	8.05	kJ/mol	Joback Method
hvap	37.33	kJ/mol	Joback Method
log10ws	-3.34		Crippen Method
logp	3.287		Crippen Method
mcvol	122.510	ml/mol	McGowan Method
pc	3121.00	kPa	Joback Method
tb	440.45	K	Joback Method
tc	655.93	K	Joback Method
tf	209.65	K	Joback Method
vc	0.449	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	241.73	J/mol×K	440.45	Joback Method
cpg	259.89	J/mol×K	476.36	Joback Method
cpg	277.08	J/mol×K	512.28	Joback Method
cpg	293.34	J/mol×K	548.19	Joback Method
cpg	308.69	J/mol×K	584.10	Joback Method
cpg	323.16	J/mol×K	620.01	Joback Method
cpg	336.77	J/mol×K	655.93	Joback Method
dvisc	0.0118957	Pa×s	209.65	Joback Method
dvisc	0.0035579	Pa×s	248.12	Joback Method

dvisc	0.0014714	Pa×s	286.58	Joback Method
dvisc	0.0007499	Pa×s	325.05	Joback Method
dvisc	0.0004408	Pa×s	363.52	Joback Method
dvisc	0.0002869	Pa×s	401.98	Joback Method
dvisc	0.0002012	Pa×s	440.45	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=C10494878&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
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