1,4-Cyclohexadiene, 1-ethyl-

Other names: 1-Ethyl-1,4-cyclohexadiene
Inchi: InChI=1S/C8H12/c1-2-8-6-4-3-5-7-8/h3-4,7H,2,5-6H2,1H3
InchiKey: PUQJLFYISQDJKP-UHFFFAOYSA-N
Formula: C8H12
SMILES: CCC1=CCC=CC1
Mol. weight [g/mol]: 108.18
CAS: 19841-74-8

Physical Properties

Property code	Value	Unit	Source
gf	98.93	kJ/mol	Joback Method
hf	-29.70	kJ/mol	Joback Method
hfus	9.29	kJ/mol	Joback Method
hvap	35.39	kJ/mol	Joback Method
log10ws	-2.77		Crippen Method
logp	2.673		Crippen Method
mcvol	104.120	ml/mol	McGowan Method
pc	3497.14	kPa	Joback Method
rinpol	900.00		NIST Webbook
rinpol	900.00		NIST Webbook
rinpol	900.00		NIST Webbook
rinpol	910.00		NIST Webbook
tb	409.96	K	Joback Method
tc	617.19	K	Joback Method
tf	205.58	K	Joback Method
vc	0.390	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	188.41	J/mol×K	409.96	Joback Method
cpg	202.55	J/mol×K	444.50	Joback Method
cpg	215.95	J/mol×K	479.04	Joback Method
cpg	228.62	J/mol×K	513.57	Joback Method

cpg	240.59	J/mol×K	548.11	Joback Method
cpg	251.88	J/mol×K	582.65	Joback Method
cpg	262.53	J/mol×K	617.19	Joback Method
dvisc	0.0044114	Pa×s	205.58	Joback Method
dvisc	0.0019336	Pa×s	239.64	Joback Method
dvisc	0.0010407	Pa×s	273.71	Joback Method
dvisc	0.0006425	Pa×s	307.77	Joback Method
dvisc	0.0004366	Pa×s	341.83	Joback Method
dvisc	0.0003182	Pa×s	375.90	Joback Method
dvisc	0.0002445	Pa×s	409.96	Joback Method

Sources

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=C19841748&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

Latest version available from: