Cyclohexane, 1,2-bis(methylene)-

Inchi: InChI=1S/C8H12/c1-7-5-3-4-6-8(7)2/h1-6H2
InchiKey: DYEQHQNRKZJUCT-UHFFFAOYSA-N
Formula: C8H12
SMILES: C=C1CCCCC1=C
Mol. weight [g/mol]: 108.18
CAS: 2819-48-9

Physical Properties

Property code	Value	Unit	Source
gf	154.80	kJ/mol	Joback Method
hf	34.69	kJ/mol	Joback Method
hfus	4.92	kJ/mol	Joback Method
hvap	34.46	kJ/mol	Joback Method
ie	8.90	eV	NIST Webbook
ie	8.92	eV	NIST Webbook
ie	8.92	eV	NIST Webbook
log10ws	-2.77		Crippen Method
logp	2.673		Crippen Method
mcvol	104.120	ml/mol	McGowan Method
pc	3419.86	kPa	Joback Method
tb	404.98	K	Joback Method
tc	610.19	K	Joback Method
tf	218.90	K	Joback Method
vc	0.386	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	187.67	J/mol×K	404.98	Joback Method
cpg	201.52	J/mol×K	439.18	Joback Method
cpg	214.72	J/mol×K	473.38	Joback Method
cpg	227.28	J/mol×K	507.59	Joback Method
cpg	239.22	J/mol×K	541.79	Joback Method
cpg	250.55	J/mol×K	575.99	Joback Method

cpg	261.29	J/mol×K	610.19	Joback Method
dvisc	0.0030331	Pa×s	218.90	Joback Method
dvisc	0.0015976	Pa×s	249.91	Joback Method
dvisc	0.0009695	Pa×s	280.93	Joback Method
dvisc	0.0006497	Pa×s	311.94	Joback Method
dvisc	0.0004681	Pa×s	342.95	Joback Method
dvisc	0.0003561	Pa×s	373.97	Joback Method
dvisc	0.0002825	Pa×s	404.98	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	397.20	K	98.70	NIST Webbook
tbrp	333.70	K	12.00	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2819489&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
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume