2,3-Dimethyl-cyclohexa-1,3-diene

Inchi: InChI=1S/C8H12/c1-7-5-3-4-6-8(7)2/h5-6H,3-4H2,1-2H3
InchiKey: LYIAPOCBDHFNSZ-UHFFFAOYSA-N
Formula: C8H12
SMILES: CC1=CCCC=C1C
Mol. weight [g/mol]: 108.18
CAS: 4430-91-5

Physical Properties

Property code	Value	Unit	Source
gf	89.30	kJ/mol	Joback Method
hf	-41.17	kJ/mol	Joback Method
hfus	8.91	kJ/mol	Joback Method
hvap	36.05	kJ/mol	Joback Method
log10ws	-2.77		Crippen Method
logp	2.673		Crippen Method
mcvol	104.120	ml/mol	McGowan Method
pc	3435.91	kPa	Joback Method
rinpol	856.00		NIST Webbook
tb	408.70 ± 4.00	K	NIST Webbook
tc	623.73	K	Joback Method
tf	218.10	K	Joback Method
vc	0.390	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	189.88	J/mol×K	414.94	Joback Method
cpg	251.30	J/mol×K	588.93	Joback Method
cpg	240.29	J/mol×K	554.14	Joback Method
cpg	228.67	J/mol×K	519.34	Joback Method
cpg	216.40	J/mol×K	484.54	Joback Method
cpg	203.48	J/mol×K	449.74	Joback Method
cpg	261.72	J/mol×K	623.73	Joback Method
dvisc	0.0002292	Pa×s	414.94	Joback Method

dvisc	0.0002903	Pa×s	382.13	Joback Method
dvisc	0.0003843	Pa×s	349.33	Joback Method
dvisc	0.0005393	Pa×s	316.52	Joback Method
dvisc	0.0008183	Pa×s	283.71	Joback Method
dvisc	0.0013849	Pa×s	250.91	Joback Method
dvisc	0.0027458	Pa×s	218.10	Joback Method

Sources

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=C4430915&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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