1,3,6-Heptatriene

Inchi: InChI=1S/C7H10/c1-3-5-7-6-4-2/h3-5,7H,1-2,6H2/b7-5+
InchiKey: CXHZYOISZDAYCU-FNORWQNLSA-N
Formula: C7H10
SMILES: C=CC=CCC=C
Mol. weight [g/mol]: 94.15
CAS: 1002-27-3

Physical Properties

Property code	Value	Unit	Source
gf	263.96	kJ/mol	Joback Method
hf	180.27	kJ/mol	Joback Method
hfus	11.53	kJ/mol	Joback Method
hvap	29.79	kJ/mol	Joback Method
log10ws	-2.31		Crippen Method
logp	2.305		Crippen Method
mcvol	96.590	ml/mol	McGowan Method
pc	3250.43	kPa	Joback Method
tb	357.08	K	Joback Method
tc	536.82	K	Joback Method
tf	160.05	K	Joback Method
vc	0.369	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	153.02	J/mol×K	357.08	Joback Method
cpg	163.52	J/mol×K	387.04	Joback Method
cpg	173.48	J/mol×K	416.99	Joback Method
cpg	182.91	J/mol×K	446.95	Joback Method
cpg	191.84	J/mol×K	476.91	Joback Method
cpg	200.29	J/mol×K	506.87	Joback Method
cpg	208.29	J/mol×K	536.82	Joback Method
dvisc	0.0030068	Pa×s	160.05	Joback Method
dvisc	0.0012629	Pa×s	192.89	Joback Method

dvisc	0.0006828	Pa×s	225.73	Joback Method
dvisc	0.0004315	Pa×s	258.56	Joback Method
dvisc	0.0003025	Pa×s	291.40	Joback Method
dvisc	0.0002278	Pa×s	324.24	Joback Method
dvisc	0.0001808	Pa×s	357.08	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=C1002273&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume