1,3,5-Cycloheptatriene, methyl

Inchi: InChI=1S/C8H10/c1-8-6-4-2-3-5-7-8/h2-4,6-7H,5H2,1H3
InchiKey: UQJRWEWFCRBHQV-UHFFFAOYSA-N
Formula: C8H10
SMILES: CC1=CCC=CC=C1
Mol. weight [g/mol]: 106.17

Physical Properties

Property code	Value	Unit	Source
gf	116.79	kJ/mol	Joback Method
hf	21.92	kJ/mol	Joback Method
hfus	8.42	kJ/mol	Joback Method
hvap	35.85	kJ/mol	Joback Method
log10ws	-2.63		Crippen Method
logp	2.449		Crippen Method
mcvol	99.820	ml/mol	McGowan Method
pc	3763.78	kPa	Joback Method
rinpol	890.00		NIST Webbook
rinpol	890.00		NIST Webbook
tb	413.39	K	Joback Method
tc	631.79	K	Joback Method
tf	202.82	K	Joback Method
vc	0.367	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	173.68	J/mol×K	413.39	Joback Method
cpg	187.43	J/mol×K	449.79	Joback Method
cpg	200.42	J/mol×K	486.19	Joback Method
cpg	212.66	J/mol×K	522.59	Joback Method
cpg	224.19	J/mol×K	558.99	Joback Method
cpg	235.02	J/mol×K	595.39	Joback Method
cpg	245.18	J/mol×K	631.79	Joback Method
dvisc	0.0055690	Pa×s	202.82	Joback Method

dvisc	0.0021470	Pa×s	237.91	Joback Method
dvisc	0.0010576	Pa×s	273.01	Joback Method
dvisc	0.0006122	Pa×s	308.11	Joback Method
dvisc	0.0003962	Pa×s	343.20	Joback Method
dvisc	0.0002780	Pa×s	378.29	Joback Method
dvisc	0.0002072	Pa×s	413.39	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=R128124&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