

1,3,5-Cycloheptatriene, 7-ethyl-

Other names:	7-Ethyl-1,3,5-cycloheptatriene 7-Ethylcycloheptatriene
Inchi:	InChI=1S/C9H12/c1-2-9-7-5-3-4-6-8-9/h3-9H,2H2,1H3
InchiKey:	DKCPRYXLHFWDCQ-UHFFFAOYSA-N
Formula:	C9H12
SMILES:	CCC1C=CC=CC=C1
Mol. weight [g/mol]:	120.19
CAS:	17634-51-4

Physical Properties

Property code	Value	Unit	Source
gf	127.13	kJ/mol	Joback Method
hf	-7.59	kJ/mol	Joback Method
hfus	12.47	kJ/mol	Joback Method
hvap	37.11	kJ/mol	Joback Method
log10ws	-2.80		Crippen Method
logp	2.695		Crippen Method
mcvol	113.910	ml/mol	McGowan Method
pc	3287.81	kPa	Joback Method
tb	426.62	K	Joback Method
tc	640.39	K	Joback Method
tf	197.33	K	Joback Method
vc	0.422	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	212.75	J/mol×K	426.62	Joback Method
cpg	283.59	J/mol×K	604.76	Joback Method
cpg	271.05	J/mol×K	569.14	Joback Method
cpg	257.72	J/mol×K	533.51	Joback Method
cpg	243.58	J/mol×K	497.88	Joback Method
cpg	228.60	J/mol×K	462.25	Joback Method
cpg	295.36	J/mol×K	640.39	Joback Method

dvisc	0.0002118	Paxs	426.62	Joback Method
dvisc	0.0002799	Paxs	388.40	Joback Method
dvisc	0.0003930	Paxs	350.19	Joback Method
dvisc	0.0005997	Paxs	311.98	Joback Method
dvisc	0.0010298	Paxs	273.76	Joback Method
dvisc	0.0021073	Paxs	235.54	Joback Method
dvisc	0.0056906	Paxs	197.33	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17634514&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
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

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