

(Z,Z)-1,5-Cyclooctadiene, 3-methyl

Inchi:	InChI=1S/C9H14/c1-9-7-5-3-2-4-6-8-9/h3,5-6,8-9H,2,4,7H2,1H3/b5-3-,8-6-
InchiKey:	WEPNHFXHEPXGAL-NIOMPZRHSA-N
Formula:	C9H14
SMILES:	CC1C=CCCC=CC1
Mol. weight [g/mol]:	122.21
CAS:	15840-71-8

Physical Properties

Property code	Value	Unit	Source
gf	85.07	kJ/mol	Joback Method
hf	-71.53	kJ/mol	Joback Method
hfus	9.14	kJ/mol	Joback Method
hvap	36.98	kJ/mol	Joback Method
log10ws	-2.95		Crippen Method
logp	2.919		Crippen Method
mcvol	118.210	ml/mol	McGowan Method
pc	3246.73	kPa	Joback Method
rinpol	978.00		NIST Webbook
tb	431.73	K	Joback Method
tc	652.12	K	Joback Method
tf	193.05	K	Joback Method
vc	0.428	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	225.74	J/molxK	431.73	Joback Method
cpg	243.99	J/molxK	468.46	Joback Method
cpg	261.29	J/molxK	505.19	Joback Method
cpg	277.65	J/molxK	541.92	Joback Method
cpg	293.10	J/molxK	578.66	Joback Method
cpg	307.64	J/molxK	615.39	Joback Method
cpg	321.29	J/molxK	652.12	Joback Method
dvisc	0.0149019	Paxs	193.05	Joback Method

dvisc	0.0038907	Paxs	232.83	Joback Method
dvisc	0.0015032	Paxs	272.61	Joback Method
dvisc	0.0007399	Paxs	312.39	Joback Method
dvisc	0.0004275	Paxs	352.17	Joback Method
dvisc	0.0002761	Paxs	391.95	Joback Method
dvisc	0.0001932	Paxs	431.73	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C15840718&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
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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