(Z,E,E)-2,4,6-nonatriene

Inchi: InChI=1S/C9H14/c1-3-5-7-9-8-6-4-2/h3,5-9H,4H2,1-2H3/b5-3-,8-6+,9-7+
InchiKey: QTRAFXCHKGPQFY-JKNUXMOISA-N
Formula: C9H14
SMILES: CC=CC=CC=CCC
Mol. weight [g/mol]: 122.21

Physical Properties

Property code	Value	Unit	Source
gf	265.56	kJ/mol	Joback Method
hf	122.57	kJ/mol	Joback Method
hfus	19.67	kJ/mol	Joback Method
hvap	35.50	kJ/mol	Joback Method
log10ws	-3.15		Crippen Method
logp	3.085		Crippen Method
mcvol	124.770	ml/mol	McGowan Method
pc	2695.80	kPa	Joback Method
ripol	1239.00		NIST Webbook
tb	417.80	K	Joback Method
tc	606.70	K	Joback Method
tf	175.95	K	Joback Method
vc	0.479	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	228.22	J/mol×K	417.80	Joback Method
cpg	241.80	J/mol×K	449.28	Joback Method
cpg	254.60	J/mol×K	480.77	Joback Method
cpg	266.65	J/mol×K	512.25	Joback Method
cpg	278.00	J/mol×K	543.73	Joback Method
cpg	288.71	J/mol×K	575.22	Joback Method
cpg	298.80	J/mol×K	606.70	Joback Method
dvisc	0.0049437	Pa×s	175.95	Joback Method
dvisc	0.0015637	Pa×s	216.26	Joback Method

dvisc	0.0007101	Pa×s	256.57	Joback Method
dvisc	0.0003996	Pa×s	296.88	Joback Method
dvisc	0.0002580	Pa×s	337.18	Joback Method
dvisc	0.0001829	Pa×s	377.49	Joback Method
dvisc	0.0001385	Pa×s	417.80	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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=R301196&Units=SI

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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume