1,7-Octadiene, 2-methyl

Other names: 2-Methyl-1,7-octadiene
Inchi: InChI=1S/C9H16/c1-4-5-6-7-8-9(2)3/h4H,1-2,5-8H2,3H3
InchiKey: GRMXFZGBPICEAU-UHFFFAOYSA-N
Formula: C9H16
SMILES: C=CCCCCC(=C)C
Mol. weight [g/mol]: 124.22

Physical Properties

Property code	Value	Unit	Source
gf	192.03	kJ/mol	Joback Method
hf	11.98	kJ/mol	Joback Method
hfus	15.20	kJ/mol	Joback Method
hvap	34.37	kJ/mol	Joback Method
log10ws	-3.30		Crippen Method
logp	3.309		Crippen Method
mcvol	129.070	ml/mol	McGowan Method
pc	2517.59	kPa	Joback Method
rinpol	850.00		NIST Webbook
rinpol	857.00		NIST Webbook
rinpol	857.00		NIST Webbook
rinpol	857.00		NIST Webbook
rinpol	850.00		NIST Webbook
rinpol	850.00		NIST Webbook
tb	398.56	K	Joback Method
tc	571.52	K	Joback Method
tf	173.71	K	Joback Method
vc	0.502	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	242.10	J/mol×K	398.56	Joback Method
cpg	255.42	J/mol×K	427.39	Joback Method
cpg	268.17	J/mol×K	456.21	Joback Method

cpg	280.36	J/mol×K	485.04	Joback Method
cpg	292.03	J/mol×K	513.87	Joback Method
cpg	303.17	J/mol×K	542.69	Joback Method
cpg	313.83	J/mol×K	571.52	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R1939&Units=SI
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

Legend

cpg:	Ideal gas heat capacity
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