3-methyl-1,7-octadiene

Other names: 1,7-Octadiene, 3-methyl
Inchi: InChI=1S/C9H16/c1-4-6-7-8-9(3)5-2/h4-5,9H,1-2,6-8H2,3H3
InchiKey: LFXNEGVBUADMEB-UHFFFAOYSA-N
Formula: C9H16
SMILES: C=CCCCC(C)C=C
Mol. weight [g/mol]: 124.22

Physical Properties

Property code	Value	Unit	Source
gf	198.14	kJ/mol	Joback Method
hf	16.49	kJ/mol	Joback Method
hfus	12.98	kJ/mol	Joback Method
hvap	33.90	kJ/mol	Joback Method
log10ws	-3.06		Crippen Method
logp	3.165		Crippen Method
mcvol	129.070	ml/mol	McGowan Method
pc	2525.19	kPa	Joback Method
rinpol	821.00		NIST Webbook
rinpol	823.00		NIST Webbook
rinpol	823.00		NIST Webbook
rinpol	823.00		NIST Webbook
rinpol	830.00		NIST Webbook
rinpol	821.00		NIST Webbook
rinpol	821.00		NIST Webbook
tb	398.24	K	Joback Method
tc	571.80	K	Joback Method
tf	172.67	K	Joback Method
vc	0.495	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	242.06	J/mol×K	398.24	Joback Method
cpg	255.55	J/mol×K	427.17	Joback Method

cpg	268.46	J/mol×K	456.09	Joback Method
cpg	280.80	J/mol×K	485.02	Joback Method
cpg	292.60	J/mol×K	513.95	Joback Method
cpg	303.88	J/mol×K	542.87	Joback Method
cpg	314.64	J/mol×K	571.80	Joback Method
dvisc	0.0074402	Pa×s	172.67	Joback Method
dvisc	0.0024687	Pa×s	210.27	Joback Method
dvisc	0.0011447	Pa×s	247.86	Joback Method
dvisc	0.0006499	Pa×s	285.46	Joback Method
dvisc	0.0004209	Pa×s	323.05	Joback Method
dvisc	0.0002985	Pa×s	360.64	Joback Method
dvisc	0.0002258	Pa×s	398.24	Joback Method

Sources

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=R1942&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

Latest version available from:
https://www.chemeo.com/cid/63-662-7/3-methyl-1-7-octadiene.pdf
Generated by Cheméo on 2024-04-27 03:58:46.564488016 +0000 UTC m=+16479575.485065376.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.