1,5-Octadiene, 7-methyl-3-(1-methylethyl)-

Inchi: InChI=1S/C12H22/c1-6-12(11(4)5)9-7-8-10(2)3/h6-8,10-12H,1,9H2,2-5H3/b8-7+
InchiKey: FILKYXIIUVXJQM-BQYQJAHWSA-N
Formula: C12H22
SMILES: C=CC(CC=CC(C)C)C(C)C
Mol. weight [g/mol]: 166.30
CAS: 74630-12-9

Physical Properties

Property code	Value	Unit	Source
gf	210.90	kJ/mol	Joback Method
hf	-64.20	kJ/mol	Joback Method
hfus	15.19	kJ/mol	Joback Method
hvap	40.43	kJ/mol	Joback Method
log10ws	-3.83		Crippen Method
logp	4.047		Crippen Method
mcvol	171.340	ml/mol	McGowan Method
pc	1971.80	kPa	Joback Method
tb	473.48	K	Joback Method
tc	655.84	K	Joback Method
tf	173.16	K	Joback Method
vc	0.650	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	373.35	J/mol×K	473.48	Joback Method
cpg	390.76	J/mol×K	503.87	Joback Method
cpg	407.34	J/mol×K	534.27	Joback Method
cpg	423.12	J/mol×K	564.66	Joback Method
cpg	438.13	J/mol×K	595.05	Joback Method
cpg	452.40	J/mol×K	625.45	Joback Method
cpg	465.98	J/mol×K	655.84	Joback Method
dvisc	0.0331288	Pa×s	173.16	Joback Method
dvisc	0.0049698	Pa×s	223.21	Joback Method

dvisc	0.0014938	Pa×s	273.27	Joback Method
dvisc	0.0006514	Pa×s	323.32	Joback Method
dvisc	0.0003549	Pa×s	373.37	Joback Method
dvisc	0.0002232	Pa×s	423.43	Joback Method
dvisc	0.0001548	Pa×s	473.48	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=C74630129&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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume