2-Methyl-2,4,6-octatriene

Inchi: InChI=1S/C9H14/c1-4-5-6-7-8-9(2)3/h4-8H,1-3H3/b5-4+,7-6+
InchiKey: AHXXJOUHGBPWGW-YTXTXJHMSA-N
Formula: C9H14
SMILES: CC=CC=CC=C(C)C
Mol. weight [g/mol]: 122.21

Physical Properties

Property code	Value	Unit	Source
gf	257.01	kJ/mol	Joback Method
hf	112.78	kJ/mol	Joback Method
hfus	18.36	kJ/mol	Joback Method
hvap	35.58	kJ/mol	Joback Method
log10ws	-3.15		Crippen Method
logp	3.085		Crippen Method
mcvol	124.770	ml/mol	McGowan Method
pc	2709.85	kPa	Joback Method
rinpol	985.00		NIST Webbook
rinpol	985.00		NIST Webbook
tb	417.68	K	Joback Method
tc	610.37	K	Joback Method
tf	161.99	K	Joback Method
vc	0.480	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	228.18	J/mol×K	417.68	Joback Method
cpg	241.99	J/mol×K	449.79	Joback Method
cpg	254.98	J/mol×K	481.91	Joback Method
cpg	267.21	J/mol×K	514.02	Joback Method
cpg	278.72	J/mol×K	546.14	Joback Method
cpg	289.55	J/mol×K	578.25	Joback Method
cpg	299.75	J/mol×K	610.37	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R591225&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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