2,6-Dimethyl-1,3,6-heptatriene

Inchi: InChI=1S/C9H14/c1-8(2)6-5-7-9(3)4/h5-6H,1,3,7H2,2,4H3/b6-5+
InchiKey: BEVRACFYDJMTEY-AATRIKPKSA-N
Formula: C9H14
SMILES: C=C(C)C=CCC(=C)C
Mol. weight [g/mol]: 122.21
CAS: 928-67-6

Physical Properties

Property code	Value	Unit	Source
gf	263.70	kJ/mol	Joback Method
hf	119.41	kJ/mol	Joback Method
hfus	14.09	kJ/mol	Joback Method
hvap	34.41	kJ/mol	Joback Method
log10ws	-3.15		Crippen Method
logp	3.085		Crippen Method
mcvol	124.770	ml/mol	McGowan Method
pc	2668.02	kPa	Joback Method
tb	402.60	K	Joback Method
tc	588.08	K	Joback Method
tf	154.67	K	Joback Method
vc	0.483	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	227.40	J/mol×K	402.60	Joback Method
cpg	240.77	J/mol×K	433.51	Joback Method
cpg	253.43	J/mol×K	464.43	Joback Method
cpg	265.44	J/mol×K	495.34	Joback Method
cpg	276.81	J/mol×K	526.25	Joback Method
cpg	287.59	J/mol×K	557.17	Joback Method
cpg	297.80	J/mol×K	588.08	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C928676&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume