1,6-Heptadiene, 2,5-dimethyl-

Other names: 2,5-Dimethyl-1,6-heptadiene
Inchi: InChI=1S/C9H16/c1-5-9(4)7-6-8(2)3/h5,9H,1-2,6-7H2,3-4H3
InchiKey: QDURDEDFGSDOQY-UHFFFAOYSA-N
Formula: C9H16
SMILES: C=CC(C)CCC(=C)C
Mol. weight [g/mol]: 124.22
CAS: 68701-90-6

Physical Properties

Property code	Value	Unit	Source
gf	189.59	kJ/mol	Joback Method
hf	6.70	kJ/mol	Joback Method
hfus	11.67	kJ/mol	Joback Method
hvap	33.98	kJ/mol	Joback Method
log10ws	-3.06		Crippen Method
logp	3.165		Crippen Method
mcvol	129.070	ml/mol	McGowan Method
pc	2537.93	kPa	Joback Method
rinpol	1228.00		NIST Webbook
tb	398.12	K	Joback Method
tc	575.10	K	Joback Method
tf	158.71	K	Joback Method
vc	0.496	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	242.03	J/mol×K	398.12	Joback Method
cpg	255.75	J/mol×K	427.62	Joback Method
cpg	268.86	J/mol×K	457.11	Joback Method
cpg	281.39	J/mol×K	486.61	Joback Method
cpg	293.36	J/mol×K	516.10	Joback Method
cpg	304.78	J/mol×K	545.60	Joback Method
cpg	315.68	J/mol×K	575.10	Joback Method

Sources

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=C68701906&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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