6-Methyl-3,5-heptadienone

Inchi: InChI=1S/C8H12O/c1-7(2)5-4-6-8(3)9/h4-6H,1-3H3/b6-4+
InchiKey: KSKXSFZGARKWOW-GQCTYLIASA-N
Formula: C8H12O
SMILES: CC(=O)C=CC=C(C)C
Mol. weight [g/mol]: 124.18

Physical Properties

Property code	Value	Unit	Source
gf	39.45	kJ/mol	Joback Method
hf	-96.38	kJ/mol	Joback Method
hfus	17.17	kJ/mol	Joback Method
hvap	40.14	kJ/mol	Joback Method
log10ws	-2.16		Crippen Method
logp	2.098		Crippen Method
mcvol	116.550	ml/mol	McGowan Method
pc	3038.96	kPa	Joback Method
rinpol	1102.00		NIST Webbook
rinpol	1102.00		NIST Webbook
tb	444.51	K	Joback Method
tc	641.39	K	Joback Method
tf	205.73	K	Joback Method
vc	0.451	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	223.66	J/mol×K	444.51	Joback Method
cpg	235.68	J/mol×K	477.32	Joback Method
cpg	247.03	J/mol×K	510.14	Joback Method
cpg	257.73	J/mol×K	542.95	Joback Method
cpg	267.82	J/mol×K	575.76	Joback Method
cpg	277.33	J/mol×K	608.58	Joback Method
cpg	286.31	J/mol×K	641.39	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=R587038&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