(E)-5,7-Octadien-4-one, 3,6-dimethyl

Inchi: InChI=1S/C10H16O/c1-5-8(3)7-10(11)9(4)6-2/h5,7,9H,1,6H2,2-4H3/b8-7+
InchiKey: NFUBAHYHMDPSQY-BQYQJAHWSA-N
Formula: C10H16O
SMILES: C=CC(C)=CC(=O)C(C)CC
Mol. weight [g/mol]: 152.23

Physical Properties

Property code	Value	Unit	Source
gf	61.47	kJ/mol	Joback Method
hf	-134.73	kJ/mol	Joback Method
hfus	17.34	kJ/mol	Joback Method
hvap	43.58	kJ/mol	Joback Method
log10ws	-2.75		Crippen Method
logp	2.734		Crippen Method
mcvol	144.730	ml/mol	McGowan Method
pc	2480.12	kPa	Joback Method
rinpol	1129.00		NIST Webbook
rinpol	1129.00		NIST Webbook
rinpol	1129.00		NIST Webbook
ripol	1570.00		NIST Webbook
ripol	1570.00		NIST Webbook
tb	482.35	K	Joback Method
tc	674.03	K	Joback Method
tf	216.59	K	Joback Method
vc	0.557	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	307.71	J/mol×K	482.35	Joback Method
cpg	321.86	J/mol×K	514.30	Joback Method
cpg	335.28	J/mol×K	546.24	Joback Method
cpg	347.99	J/mol×K	578.19	Joback Method
cpg	360.04	J/mol×K	610.14	Joback Method

cpg	371.44	J/mol×K	642.09	Joback Method
cpg	382.25	J/mol×K	674.03	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=R324837&Units=SI

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume