4,8-Dimethylnona-3,8-dien-2-one

Inchi: InChI=1S/C11H18O/c1-9(2)6-5-7-10(3)8-11(4)12/h8H,1,5-7H2,2-4H3/b10-8+
InchiKey: HCJMBPAWBFFIJI-CSKARUKUSA-N
Formula: C11H18O
SMILES: C=C(C)CCCC(C)=CC(C)=O
Mol. weight [g/mol]: 166.26
CAS: 872858-42-9

Physical Properties

Property code	Value	Unit	Source
gf	63.78	kJ/mol	Joback Method
hf	-159.88	kJ/mol	Joback Method
hfus	22.15	kJ/mol	Joback Method
hvap	46.27	kJ/mol	Joback Method
log10ws	-3.41		Crippen Method
logp	3.268		Crippen Method
mcvol	158.820	ml/mol	McGowan Method
pc	2252.53	kPa	Joback Method
rinpol	1275.50		NIST Webbook
tb	505.55	K	Joback Method
tc	694.38	K	Joback Method
tf	228.90	K	Joback Method
vc	0.621	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	352.30	J/mol×K	505.55	Joback Method
cpg	367.13	J/mol×K	537.02	Joback Method
cpg	381.20	J/mol×K	568.49	Joback Method
cpg	394.56	J/mol×K	599.96	Joback Method
cpg	407.23	J/mol×K	631.44	Joback Method
cpg	419.26	J/mol×K	662.91	Joback Method
cpg	430.67	J/mol×K	694.38	Joback Method

Sources

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=C872858429&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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