(2E)-2,6-dimethyl-2,5-heptadienoic acid

Inchi: InChI=1S/C9H14O2/c1-7(2)5-4-6-8(3)9(10)11/h5-6H,4H2,1-3H3,(H,10,11)/b8-6+
InchiKey: IGQGIACCENRGLM-SOFGYWHQSA-N
Formula: C9H14O2
SMILES: CC(C)=CCC=C(C)C(=O)O
Mol. weight [g/mol]: 154.21

Physical Properties

Property code	Value	Unit	Source
gf	-97.50	kJ/mol	Joback Method
hf	-279.04	kJ/mol	Joback Method
hfus	22.54	kJ/mol	Joback Method
hvap	59.13	kJ/mol	Joback Method
log10ws	-2.40		Crippen Method
logp	2.374		Crippen Method
mcvol	136.510	ml/mol	McGowan Method
pc	3042.32	kPa	Joback Method
ripol	2311.00		NIST Webbook
ripol	2311.00		NIST Webbook
tb	559.45	K	Joback Method
tc	746.72	K	Joback Method
tf	263.86	K	Joback Method
vc	0.526	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	316.53	J/mol×K	559.45	Joback Method
cpg	327.49	J/mol×K	590.66	Joback Method
cpg	337.85	J/mol×K	621.87	Joback Method
cpg	347.66	J/mol×K	653.09	Joback Method
cpg	356.94	J/mol×K	684.30	Joback Method
cpg	365.74	J/mol×K	715.51	Joback Method
cpg	374.09	J/mol×K	746.72	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=R334453&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume