2,2-DIMETHYLOCTA-3,4-DIENAL

Other names: 3,4-Octadienal, 2,2-dimethyl
2,2-Dimethyl-3,4-octadienal
Inchi: InChI=1S/C10H16O/c1-4-5-6-7-8-10(2,3)9-11/h6,8-9H,4-5H2,1-3H3
InchiKey: VSFHYKIILWBKOH-UHFFFAOYSA-N
Formula: C10H16O
SMILES: CCCC=C=CC(C)(C)C=O
Mol. weight [g/mol]: 152.24

Physical Properties

Property code	Value	Unit	Source
hfus	18.86	kJ/mol	Joback Method
logp	2.723		Crippen Method
mcvol	144.730	ml/mol	McGowan Method
rinpol	1116.00		NIST Webbook
rinpol	1098.00		NIST Webbook
rinpol	1116.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	315.27	J/mol×K	481.06	Joback Method
cpg	329.61	J/mol×K	514.08	Joback Method
cpg	343.15	J/mol×K	547.10	Joback Method
cpg	355.94	J/mol×K	580.12	Joback Method
cpg	368.01	J/mol×K	613.14	Joback Method
cpg	379.39	J/mol×K	646.15	Joback Method
cpg	390.13	J/mol×K	679.17	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C590716&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices