7-methyl-3-methyleneoct-6-enal

Inchi: InChI=1S/C10H16O/c1-9(2)5-4-6-10(3)7-8-11/h5,8H,3-4,6-7H2,1-2H3
InchiKey: ODULZPPCXSTHDT-UHFFFAOYSA-N
Formula: C10H16O
SMILES: C=C(CC=O)CCC=C(C)C
Mol. weight [g/mol]: 152.23
CAS: 55050-40-3

Physical Properties

Property code	Value	Unit	Source
gf	84.76	kJ/mol	Joback Method
hf	-112.24	kJ/mol	Joback Method
hfus	20.25	kJ/mol	Joback Method
hvap	44.02	kJ/mol	Joback Method
log10ws	-3.00		Crippen Method
logp	2.878		Crippen Method
mcvol	144.730	ml/mol	McGowan Method
pc	2500.00	kPa	Joback Method
tb	477.46	K	Joback Method
tc	663.69	K	Joback Method
tf	209.70	K	Joback Method
vc	0.576	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	308.38	J/mol×K	477.46	Joback Method
cpg	322.01	J/mol×K	508.50	Joback Method
cpg	334.96	J/mol×K	539.54	Joback Method
cpg	347.25	J/mol×K	570.58	Joback Method
cpg	358.90	J/mol×K	601.61	Joback Method
cpg	369.96	J/mol×K	632.65	Joback Method
cpg	380.46	J/mol×K	663.69	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55050403&Units=SI
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

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