2,4,6-Octatrienal

Other names: Octatrienal
Inchi: InChI=1S/C8H10O/c1-2-3-4-5-6-7-8-9/h2-8H,1H3/b3-2+,5-4+,7-6+
InchiKey: ZUZGMJKUENNLQL-ICDJNDDTSA-N
Formula: C8H10O
SMILES: CC=CC=CC=CC=O
Mol. weight [g/mol]: 122.16
CAS: 17609-31-3

Physical Properties

Property code	Value	Unit	Source
gf	157.62	kJ/mol	Joback Method
hf	57.63	kJ/mol	Joback Method
hfus	19.37	kJ/mol	Joback Method
hvap	40.00	kJ/mol	Joback Method
ie	8.42 ± 0.03	eV	NIST Webbook
log10ws	-2.01		Crippen Method
logp	1.874		Crippen Method
mcvol	112.250	ml/mol	McGowan Method
pc	3243.03	kPa	Joback Method
tb	443.58	K	Joback Method
tc	640.89	K	Joback Method
tf	206.68	K	Joback Method
vc	0.441	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	209.11	J/mol×K	443.58	Joback Method
cpg	220.20	J/mol×K	476.47	Joback Method
cpg	230.57	J/mol×K	509.35	Joback Method
cpg	240.26	J/mol×K	542.24	Joback Method
cpg	249.32	J/mol×K	575.12	Joback Method
cpg	257.79	J/mol×K	608.01	Joback Method
cpg	265.73	J/mol×K	640.89	Joback Method

dvisc	0.0039000	Pa×s	206.68	Joback Method
dvisc	0.0015547	Pa×s	246.16	Joback Method
dvisc	0.0007992	Pa×s	285.65	Joback Method
dvisc	0.0004829	Pa×s	325.13	Joback Method
dvisc	0.0003254	Pa×s	364.61	Joback Method
dvisc	0.0002369	Pa×s	404.10	Joback Method
dvisc	0.0001825	Pa×s	443.58	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	335.70	K	0.07	NIST Webbook

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=C17609313&Units=SI

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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
ie: Ionization energy
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

tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume