

4-Oxo-trans-2-octenal

Other names:	(E)-4-Oxo-2-octenal
Inchi:	InChI=1S/C8H12O2/c1-2-3-5-8(10)6-4-7-9/h4,6-7H,2-3,5H2,1H3/b6-4+
InchiKey:	KKCMFNUPOSVKRS-GQCTYLIASA-N
Formula:	C8H12O2
SMILES:	CCCCC(=O)C=CC=O
Mol. weight [g/mol]:	140.18
CAS:	2497-14-5

Physical Properties

Property code	Value	Unit	Source
gf	-131.74	kJ/mol	Joback Method
hf	-289.39	kJ/mol	Joback Method
hfus	20.57	kJ/mol	Joback Method
hvap	46.83	kJ/mol	Joback Method
log10ws	-1.59		Crippen Method
logp	1.501		Crippen Method
mcvol	122.420	ml/mol	McGowan Method
pc	3096.73	kPa	Joback Method
rinpol	1162.00		NIST Webbook
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tb	489.13	K	Joback Method
tc	678.68	K	Joback Method
tf	266.77	K	Joback Method
vc	0.486	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	259.16	J/molxK	489.13	Joback Method
cpg	308.77	J/molxK	647.09	Joback Method
cpg	299.88	J/molxK	615.50	Joback Method
cpg	290.50	J/molxK	583.91	Joback Method
cpg	280.60	J/molxK	552.31	Joback Method
cpg	270.16	J/molxK	520.72	Joback Method

cpg	317.19	J/mol×K	678.68	Joback Method
dvisc	0.0003039	Paxs	489.13	Joback Method
dvisc	0.0003894	Paxs	452.07	Joback Method
dvisc	0.0005215	Paxs	415.01	Joback Method
dvisc	0.0007396	Paxs	377.95	Joback Method
dvisc	0.0011317	Paxs	340.89	Joback Method
dvisc	0.0019210	Paxs	303.83	Joback Method
dvisc	0.0037772	Paxs	266.77	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2497145&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
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
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

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