

4-oxooctanal

Inchi:	InChI=1S/C8H14O2/c1-2-3-5-8(10)6-4-7-9/h7H,2-6H2,1H3
InchiKey:	JWSDUZPHHXIUBR-UHFFFAOYSA-N
Formula:	C8H14O2
SMILES:	CCCCC(=O)CCC=O
Mol. weight [g/mol]:	142.20

Physical Properties

Property code	Value	Unit	Source
gf	-211.96	kJ/mol	Joback Method
hf	-406.61	kJ/mol	Joback Method
hfus	20.36	kJ/mol	Joback Method
hvap	46.87	kJ/mol	Joback Method
log10ws	-1.73		Crippen Method
logp	1.725		Crippen Method
mcvol	126.720	ml/mol	McGowan Method
pc	2925.00	kPa	Joback Method
rinpol	1100.00		NIST Webbook
rinpol	1099.00		NIST Webbook
rinpol	1099.00		NIST Webbook
tb	484.97	K	Joback Method
tc	666.17	K	Joback Method
tf	271.85	K	Joback Method
vc	0.506	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	276.45	J/molxK	484.97	Joback Method
cpg	328.86	J/molxK	635.97	Joback Method
cpg	319.33	J/molxK	605.77	Joback Method
cpg	309.33	J/molxK	575.57	Joback Method
cpg	298.86	J/molxK	545.37	Joback Method
cpg	287.91	J/molxK	515.17	Joback Method
cpg	337.94	J/molxK	666.17	Joback Method

dvisc	0.0003621	Paxs	484.97	Joback Method
dvisc	0.0004626	Paxs	449.45	Joback Method
dvisc	0.0006163	Paxs	413.93	Joback Method
dvisc	0.0008664	Paxs	378.41	Joback Method
dvisc	0.0013073	Paxs	342.89	Joback Method
dvisc	0.0021692	Paxs	307.37	Joback Method
dvisc	0.0041085	Paxs	271.85	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R224430&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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