

2-Octen-4-one

Other names:	oct-2-en-4-one
Inchi:	InChI=1S/C8H14O/c1-3-5-7-8(9)6-4-2/h4,6H,3,5,7H2,1-2H3/b6-4+
InchiKey:	FMDLEUPBHMCPQV-GQCTYLIASA-N
Formula:	C8H14O
SMILES:	CC=CC(=O)CCCC
Mol. weight [g/mol]:	126.20
CAS:	4643-27-0

Physical Properties

Property code	Value	Unit	Source
gf	-32.22	kJ/mol	Joback Method
hf	-203.81	kJ/mol	Joback Method
hfus	18.28	kJ/mol	Joback Method
hvap	40.11	kJ/mol	Joback Method
log10ws	-2.30		Crippen Method
logp	2.322		Crippen Method
mcvol	120.850	ml/mol	McGowan Method
pc	2856.62	kPa	Joback Method
tb	440.47	K	Joback Method
tc	624.44	K	Joback Method
tf	224.77	K	Joback Method
vc	0.469	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	239.73	J/mol×K	440.47	Joback Method
cpg	251.92	J/mol×K	471.13	Joback Method
cpg	263.55	J/mol×K	501.79	Joback Method
cpg	274.62	J/mol×K	532.46	Joback Method
cpg	285.17	J/mol×K	563.12	Joback Method
cpg	295.21	J/mol×K	593.78	Joback Method
cpg	304.76	J/mol×K	624.44	Joback Method
dvisc	0.0040418	Paxs	224.77	Joback Method

dvisc	0.0018362	Paxs	260.72	Joback Method
dvisc	0.0010100	Paxs	296.67	Joback Method
dvisc	0.0006321	Paxs	332.62	Joback Method
dvisc	0.0004335	Paxs	368.57	Joback Method
dvisc	0.0003179	Paxs	404.52	Joback Method
dvisc	0.0002453	Paxs	440.47	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4643270&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

cp_g:	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
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	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

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