

3-Decen-5-one

Inchi:	InChI=1S/C10H18O/c1-3-5-7-9-10(11)8-6-4-2/h6,8H,3-5,7,9H2,1-2H3/b8-6+
InchiKey:	IWQQYVVVAYYANSF-SOFGYWHQSA-N
Formula:	C10H18O
SMILES:	CCC=CC(=O)CCCC
Mol. weight [g/mol]:	154.25
CAS:	32064-73-6

Physical Properties

Property code	Value	Unit	Source
gf	-15.38	kJ/mol	Joback Method
hf	-245.09	kJ/mol	Joback Method
hfus	23.46	kJ/mol	Joback Method
hvap	44.56	kJ/mol	Joback Method
log10ws	-3.14		Crippen Method
logp	3.102		Crippen Method
mcvol	149.030	ml/mol	McGowan Method
pc	2349.64	kPa	Joback Method
rinpol	1349.50		NIST Webbook
rinpol	1349.50		NIST Webbook
tb	486.23	K	Joback Method
tc	666.81	K	Joback Method
tf	247.31	K	Joback Method
vc	0.582	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	325.30	J/mol×K	486.23	Joback Method
cpg	339.42	J/mol×K	516.33	Joback Method
cpg	352.89	J/mol×K	546.42	Joback Method
cpg	365.74	J/mol×K	576.52	Joback Method
cpg	377.98	J/mol×K	606.62	Joback Method
cpg	389.65	J/mol×K	636.71	Joback Method
cpg	400.76	J/mol×K	666.81	Joback Method

dvisc	0.0042181	Paxs	247.31	Joback Method
dvisc	0.0018451	Paxs	287.13	Joback Method
dvisc	0.0009872	Paxs	326.95	Joback Method
dvisc	0.0006050	Paxs	366.77	Joback Method
dvisc	0.0004081	Paxs	406.59	Joback Method
dvisc	0.0002953	Paxs	446.41	Joback Method
dvisc	0.0002253	Paxs	486.23	Joback Method

Sources

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=C32064736&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
mvol:	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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