

8-methylNonan-2-one

Inchi:	InChI=1S/C10H20O/c1-9(2)7-5-4-6-8-10(3)11/h9H,4-8H2,1-3H3
InchiKey:	QVXVZMFDDPTNBK-UHFFFAOYSA-N
Formula:	C10H20O
SMILES:	CC(=O)CCCCC(C)C
Mol. weight [g/mol]:	156.27

Physical Properties

Property code	Value	Unit	Source
gf	-98.04	kJ/mol	Joback Method
hf	-367.59	kJ/mol	Joback Method
hfus	19.73	kJ/mol	Joback Method
hvap	44.21	kJ/mol	Joback Method
log10ws	-3.05		Crippen Method
logp	3.182		Crippen Method
mcvol	153.330	ml/mol	McGowan Method
pc	2252.53	kPa	Joback Method
rinpol	1158.00		NIST Webbook
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tb	481.63	K	Joback Method
tc	658.01	K	Joback Method
tf	237.39	K	Joback Method
vc	0.596	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	342.14	J/mol×K	481.63	Joback Method
cpg	356.94	J/mol×K	511.03	Joback Method
cpg	371.13	J/mol×K	540.42	Joback Method
cpg	384.72	J/mol×K	569.82	Joback Method
cpg	397.72	J/mol×K	599.22	Joback Method
cpg	410.16	J/mol×K	628.61	Joback Method
cpg	422.05	J/mol×K	658.01	Joback Method
dvisc	0.0067728	Pa×s	237.39	Joback Method

dvisc	0.0026268	Pa×s	278.10	Joback Method
dvisc	0.0012976	Pa×s	318.80	Joback Method
dvisc	0.0007520	Pa×s	359.51	Joback Method
dvisc	0.0004869	Pa×s	400.22	Joback Method
dvisc	0.0003417	Pa×s	440.92	Joback Method
dvisc	0.0002545	Pa×s	481.63	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R513814&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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