9-methyldecan-3-one

Inchi: InChI=1S/C11H22O/c1-4-11(12)9-7-5-6-8-10(2)3/h10H,4-9H2,1-3H3
InchiKey: UMUMYGFFTAWUQZ-UHFFFAOYSA-N
Formula: C11H22O
SMILES: CCC(=O)CCCCCC(C)C
Mol. weight [g/mol]: 170.29

Physical Properties

Property code	Value	Unit	Source
gf	-89.62	kJ/mol	Joback Method
hf	-388.23	kJ/mol	Joback Method
hfus	22.32	kJ/mol	Joback Method
hvap	46.44	kJ/mol	Joback Method
log10ws	-3.47		Crippen Method
logp	3.572		Crippen Method
mcvol	167.420	ml/mol	McGowan Method
pc	2060.49	kPa	Joback Method
rinpol	1260.00		NIST Webbook
rinpol	1260.00		NIST Webbook
tb	504.51	K	Joback Method
tc	679.38	K	Joback Method
tf	248.66	K	Joback Method
vc	0.651	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	388.41	J/mol×K	504.51	Joback Method
cpg	460.10	J/mol×K	650.23	Joback Method
cpg	446.99	J/mol×K	621.09	Joback Method
cpg	433.29	J/mol×K	591.94	Joback Method
cpg	418.97	J/mol×K	562.80	Joback Method
cpg	404.02	J/mol×K	533.65	Joback Method
cpg	472.61	J/mol×K	679.38	Joback Method
dvisc	0.0002371	Pa×s	504.51	Joback Method

dvisc	0.0003195	Pa×s	461.87	Joback Method
dvisc	0.0004574	Pa×s	419.23	Joback Method
dvisc	0.0007105	Pa×s	376.59	Joback Method
dvisc	0.0012349	Pa×s	333.94	Joback Method
dvisc	0.0025234	Pa×s	291.30	Joback Method
dvisc	0.0065882	Pa×s	248.66	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R405451&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