

5-Decanone, 2-methyl-

Other names:	2-Methyl-5-decanone
Inchi:	InChI=1S/C11H22O/c1-4-5-6-7-11(12)9-8-10(2)3/h10H,4-9H2,1-3H3
InchiKey:	CDCHBGBDDXRJKB-UHFFFAOYSA-N
Formula:	C11H22O
SMILES:	CCCCC(=O)CCC(C)C
Mol. weight [g/mol]:	170.29
CAS:	54410-89-8

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
tb	504.51	K	Joback Method
tc	679.38	K	Joback Method
tf	248.66	K	Joback Method
vc	0.651	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0003195	Paxs	461.87	Joback Method
dvisc	0.0004574	Paxs	419.23	Joback Method
dvisc	0.0007105	Paxs	376.59	Joback Method
dvisc	0.0012349	Paxs	333.94	Joback Method
dvisc	0.0025234	Paxs	291.30	Joback Method
dvisc	0.0065882	Paxs	248.66	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.45783e+01
Coeff. B	-4.18822e+03
Coeff. C	-7.76060e+01
Temperature range (K), min.	370.68
Temperature range (K), max.	529.57

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C54410898&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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

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
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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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