

Methyl lavender ketone

Other names:	1-hydroxydecan-3-one
Inchi:	InChI=1S/C10H20O2/c1-2-3-4-5-6-7-10(12)8-9-11/h11H,2-9H2,1H3
InchiKey:	XDFCZUMLNOYCH-UHFFFAOYSA-N
Formula:	C10H20O2
SMILES:	CCCCCCCC(=O)CCO
Mol. weight [g/mol]:	172.26
CAS:	67633-95-8

Physical Properties

Property code	Value	Unit	Source
gf	-232.42	kJ/mol	Joback Method
hf	-514.54	kJ/mol	Joback Method
hfus	27.34	kJ/mol	Joback Method
hvap	61.28	kJ/mol	Joback Method
log10ws	-2.55		Crippen Method
logp	2.298		Crippen Method
mcvol	159.200	ml/mol	McGowan Method
pc	2443.48	kPa	Joback Method
rinpol	1341.00		NIST Webbook
ripol	2067.00		NIST Webbook
tb	574.25	K	Joback Method
tc	741.22	K	Joback Method
tf	313.21	K	Joback Method
vc	0.621	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	402.78	J/molxK	574.25	Joback Method
cpg	415.22	J/molxK	602.08	Joback Method
cpg	427.13	J/molxK	629.91	Joback Method
cpg	438.54	J/molxK	657.73	Joback Method
cpg	449.45	J/molxK	685.56	Joback Method
cpg	459.89	J/molxK	713.39	Joback Method

cpg	469.86	J/molxK	741.22	Joback Method
dvisc	0.0111394	Paxs	313.21	Joback Method
dvisc	0.0031819	Paxs	356.72	Joback Method
dvisc	0.0011935	Paxs	400.22	Joback Method
dvisc	0.0005426	Paxs	443.73	Joback Method
dvisc	0.0002839	Paxs	487.24	Joback Method
dvisc	0.0001652	Paxs	530.74	Joback Method
dvisc	0.0001044	Paxs	574.25	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C67633958&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

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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