

(S)-9-methyldecan-3-ol

Inchi:	InChI=1S/C11H24O/c1-4-11(12)9-7-5-6-8-10(2)3/h10-12H,4-9H2,1-3H3/t11-/m1/s1
InchiKey:	GVNZAPCZQSDLGP-LLVKDONJSA-N
Formula:	C11H24O
SMILES:	CCC(O)CCCCC(C)C
Mol. weight [g/mol]:	172.31

Physical Properties

Property code	Value	Unit	Source
gf	-99.96	kJ/mol	Joback Method
hf	-433.16	kJ/mol	Joback Method
hfus	21.29	kJ/mol	Joback Method
hvap	55.98	kJ/mol	Joback Method
log10ws	-3.56		Crippen Method
logp	3.364		Crippen Method
mcvol	171.720	ml/mol	McGowan Method
pc	2131.49	kPa	Joback Method
rinsol	1273.00		NIST Webbook
tb	542.38	K	Joback Method
tc	705.81	K	Joback Method
tf	244.55	K	Joback Method
vc	0.658	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	429.18	J/molxK	542.38	Joback Method
cpg	443.73	J/molxK	569.62	Joback Method
cpg	457.69	J/molxK	596.86	Joback Method
cpg	471.09	J/molxK	624.10	Joback Method
cpg	483.93	J/molxK	651.33	Joback Method
cpg	496.25	J/molxK	678.57	Joback Method
cpg	508.04	J/molxK	705.81	Joback Method
dvisc	0.1063589	Paxs	244.55	Joback Method
dvisc	0.0121747	Paxs	294.19	Joback Method

dvisc	0.0026058	Paxs	343.83	Joback Method
dvisc	0.0008229	Paxs	393.47	Joback Method
dvisc	0.0003364	Paxs	443.10	Joback Method
dvisc	0.0001647	Paxs	492.74	Joback Method
dvisc	0.0000919	Paxs	542.38	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R405471&Units=SI

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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