1-Decanol, 9-methyl-

Other names: 9-methyldecan-1-ol
Inchi: InChI=1S/C11H24O/c1-11(2)9-7-5-3-4-6-8-10-12/h11-12H,3-10H2,1-2H3
InchiKey: JTKHUJNVHQWSAY-UHFFFAOYSA-N
Formula: C11H24O
SMILES: CC(C)CCCCCCCCO
Mol. weight [g/mol]: 172.31
CAS: 55505-28-7

Physical Properties

Property code	Value	Unit	Source
gf	-97.52	kJ/mol	Joback Method
hf	-427.88	kJ/mol	Joback Method
hfus	24.81	kJ/mol	Joback Method
hvap	56.37	kJ/mol	Joback Method
log10ws	-3.45		Crippen Method
logp	3.365		Crippen Method
mcvol	171.720	ml/mol	McGowan Method
pc	2115.83	kPa	Joback Method
rinpol	1339.00		NIST Webbook
rinpol	1337.00		NIST Webbook
rinpol	1337.00		NIST Webbook
tb	542.82	K	Joback Method
tc	703.49	K	Joback Method
tf	259.55	K	Joback Method
vc	0.664	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	428.91	J/mol×K	542.82	Joback Method
cpg	494.72	J/mol×K	676.71	Joback Method
cpg	482.61	J/mol×K	649.93	Joback Method
cpg	469.99	J/mol×K	623.16	Joback Method
cpg	456.84	J/mol×K	596.38	Joback Method

cpg	443.16	J/mol×K	569.60	Joback Method
cpg	506.33	J/mol×K	703.49	Joback Method
dvisc	0.0000976	Pa×s	542.82	Joback Method
dvisc	0.0001682	Pa×s	495.61	Joback Method
dvisc	0.0003252	Pa×s	448.40	Joback Method
dvisc	0.0007343	Pa×s	401.18	Joback Method
dvisc	0.0020606	Pa×s	353.97	Joback Method
dvisc	0.0079438	Pa×s	306.76	Joback Method
dvisc	0.0500348	Pa×s	259.55	Joback Method

Sources

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=C55505287&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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