

2-Octen-1-ol, 3,7-dimethyl-, E

Inchi:	InChI=1S/C10H20O/c1-9(2)5-4-6-10(3)7-8-11/h7,9,11H,4-6,8H2,1-3H3/b10-7+
InchiKey:	JNAWJUOCXKIHG-JXMROGBWSA-N
Formula:	C10H20O
SMILES:	CC(=CCO)CCCC(C)C
Mol. weight [g/mol]:	156.27

Physical Properties

Property code	Value	Unit	Source
gf	-34.27	kJ/mol	Joback Method
hf	-299.81	kJ/mol	Joback Method
hfus	21.11	kJ/mol	Joback Method
hvap	54.18	kJ/mol	Joback Method
log10ws	-2.88		Crippen Method
logp	2.751		Crippen Method
mcvol	153.330	ml/mol	McGowan Method
pc	2448.32	kPa	Joback Method
rinpol	1172.00		NIST Webbook
ripol	1759.00		NIST Webbook
tb	523.98	K	Joback Method
tc	694.42	K	Joback Method
tf	229.24	K	Joback Method
vc	0.590	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	362.91	J/mol×K	523.98	Joback Method
cpg	376.24	J/mol×K	552.39	Joback Method
cpg	388.99	J/mol×K	580.79	Joback Method
cpg	401.17	J/mol×K	609.20	Joback Method
cpg	412.81	J/mol×K	637.61	Joback Method
cpg	423.93	J/mol×K	666.01	Joback Method
cpg	434.56	J/mol×K	694.42	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R294989&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
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
rinpola:	Non-polar retention indices
ripola:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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