

2-OCTANOL, 2,6-DIMETHYL-

Other names:	2,6-Dimethyl-2-octanol Tetrahydro myrcenol 2,6-dimethyloctan-2-ol
Inchi:	InChI=1S/C10H22O/c1-5-9(2)7-6-8-10(3,4)11/h9,11H,5-8H2,1-4H3
InchiKey:	WRFXXJKURVTLSY-UHFFFAOYSA-N
Formula:	C10H22O
SMILES:	CCC(C)CCCC(C)(C)O
Mol. weight [g/mol]:	158.29

Physical Properties

Property code	Value	Unit	Source
af	0.6685		Cheméo Relay (1.0)
gf	-103.10	kJ/mol	Joback Method
hf	-462.75	kJ/mol	Cheméo Relay (1.0)
hfus	14.81	kJ/mol	Joback Method
hvap	68.17	kJ/mol	Cheméo Relay (1.0)
log10ws	-2.87		Cheméo Relay (1.0)
logp	2.974		Crippen Method
mcvol	157.630	ml/mol	McGowan Method
pc	2358.78	kPa	Joback Method
rinpol	1088.60		NIST Webbook
rinpol	1090.00		NIST Webbook
rinpol	1089.00		NIST Webbook
rinpol	1090.00		NIST Webbook
rinpol	1067.00		NIST Webbook
rinpol	1089.00		NIST Webbook
ripol	1449.00		NIST Webbook
ripol	1414.00		NIST Webbook
ripol	1449.00		NIST Webbook
ripol	1414.00		NIST Webbook
tb	469.98	K	Cheméo Relay (1.0)
tc	643.68	K	Cheméo Relay (1.0)
tf	241.13	K	Cheméo Relay (1.0)
vc	0.587	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	383.78	J/mol×K	516.71	Joback Method
cpg	460.72	J/mol×K	686.53	Joback Method
cpg	449.39	J/mol×K	658.22	Joback Method
cpg	437.50	J/mol×K	629.92	Joback Method
cpg	425.02	J/mol×K	601.62	Joback Method
cpg	411.92	J/mol×K	573.32	Joback Method
cpg	398.19	J/mol×K	545.01	Joback Method
dvisc	0.0010052	Pa×s	383.71	Joback Method
dvisc	0.0001136	Pa×s	516.71	Joback Method
dvisc	0.0002050	Pa×s	472.38	Joback Method
dvisc	0.0004181	Pa×s	428.04	Joback Method
dvisc	0.0899105	Pa×s	250.70	Joback Method
dvisc	0.0030395	Pa×s	339.37	Joback Method
dvisc	0.0128169	Pa×s	295.03	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C18479577&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af:	Acentric Factor
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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