

4-OCTENE-2,7-DIOL, 2,7-DIMETHYL-, Z-

Other names:	cis-2,7-Dimethyl-4-octene-2,7-diol
Inchi:	InChI=1S/C10H20O2/c1-9(2,11)7-5-6-8-10(3,4)12/h5-6,11-12H,7-8H2,1-4H3/b6-5+
InchiKey:	LQBJEGDVJSXOJN-WAYWQWQTSA-N
Formula:	C10H20O2
SMILES:	CC(C)(O)C/C=C\C(C)C(C)O
Mol. weight [g/mol]:	172.27

Physical Properties

Property code	Value	Unit	Source
hf	-542.37	kJ/mol	Cheméo Relay (1.0)
hfus	15.21	kJ/mol	Joback Method
hvap	86.94	kJ/mol	Cheméo Relay (1.0)
ie	9.14	eV	Cheméo Relay (1.0)
log10ws	-1.34		Cheméo Relay (1.0)
logp	1.865		Crippen Method
mcvol	159.200	ml/mol	McGowan Method
pc	2758.46	kPa	Joback Method
tb	505.76	K	Cheméo Relay (1.0)
tc	682.61	K	Cheméo Relay (1.0)
tf	300.01	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	427.47	J/mol×K	610.26	Joback Method
cpg	439.38	J/mol×K	639.54	Joback Method
cpg	450.60	J/mol×K	668.83	Joback Method
cpg	461.19	J/mol×K	698.11	Joback Method
cpg	471.19	J/mol×K	727.40	Joback Method
cpg	480.66	J/mol×K	756.68	Joback Method
cpg	489.64	J/mol×K	785.97	Joback Method
dvisc	0.0329250	Pa×s	323.86	Joback Method
dvisc	0.0042721	Pa×s	371.59	Joback Method
dvisc	0.0008824	Pa×s	419.33	Joback Method

dvisc	0.0002516	Pa×s	467.06	Joback Method
dvisc	0.0000905	Pa×s	514.79	Joback Method
dvisc	0.0000387	Pa×s	562.53	Joback Method
dvisc	0.0000189	Pa×s	610.26	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U151608&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

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