7-Octen-2-ol

Inchi:	InChI=1S/C8H16O/c1-3-4-5-6-7-8(2)9/h3,8-9H,1,4-7H2,2H3
InchiKey:	HSHUHVOEMVTVRS-UHFFFAOYSA-N
Formula:	C8H16O
SMILES:	C=CCCCCC(C)O
Mol. weight [g/mol]:	128.21
CAS:	39546-75-3

Physical Properties

Property code	Value	Unit	Source
gf	-34.94	kJ/mol	Joback Method
hf	-240.53	kJ/mol	Joback Method
hfus	15.76	kJ/mol	Joback Method
hvap	49.02	kJ/mol	Joback Method
log10ws	-2.40		Crippen Method
logp	2.114		Crippen Method
mcvol	125.150	ml/mol	McGowan Method
pc	2940.89	kPa	Joback Method
rinpol	1064.00		NIST Webbook
rinpol	1064.00		NIST Webbook
tb	470.86	K	Joback Method
tc	636.76	K	Joback Method
tf	223.98	K	Joback Method
vc	0.477	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	273.08	J/mol×K	470.86	Joback Method
cpg	284.36	J/mol×K	498.51	Joback Method
cpg	295.19	J/mol×K	526.16	Joback Method
cpg	305.56	J/mol×K	553.81	Joback Method
cpg	315.50	J/mol×K	581.46	Joback Method
cpg	325.02	J/mol×K	609.11	Joback Method
cpg	334.14	J/mol×K	636.76	Joback Method

dvisc	0.1097275	Pa×s	223.98	Joback Method
dvisc	0.0162547	Pa×s	265.13	Joback Method
dvisc	0.0040223	Pa×s	306.27	Joback Method
dvisc	0.0013856	Pa×s	347.42	Joback Method
dvisc	0.0005982	Pa×s	388.57	Joback Method
dvisc	0.0003033	Pa×s	429.71	Joback Method
dvisc	0.0001732	Pa×s	470.86	Joback Method

Sources

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=C39546753&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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