3-Octen-2-ol

Other names: oct-3-en-2-ol
Inchi: InChI=1S/C8H16O/c1-3-4-5-6-7-8(2)9/h6-9H,3-5H2,1-2H3/b7-6+
InchiKey: YJJIVDCKSZMHGZ-VOTSOKGWSA-N
Formula: C8H16O
SMILES: CCCCC=CC(C)O
Mol. weight [g/mol]: 128.21
CAS: 76649-14-4

Physical Properties

Property code	Value	Unit	Source
gf	-42.56	kJ/mol	Joback Method
hf	-248.74	kJ/mol	Joback Method
hfus	17.24	kJ/mol	Joback Method
hvap	49.65	kJ/mol	Joback Method
log10ws	-2.40		Crippen Method
logp	2.114		Crippen Method
mcvol	125.150	ml/mol	McGowan Method
pc	2973.04	kPa	Joback Method
ripol	1769.00		NIST Webbook
ripol	1769.00		NIST Webbook
tb	478.34	K	Joback Method
tc	648.44	K	Joback Method
tf	220.66	K	Joback Method
vc	0.476	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	273.48	J/mol×K	478.34	Joback Method
cpg	326.05	J/mol×K	620.09	Joback Method
cpg	316.47	J/mol×K	591.74	Joback Method
cpg	306.45	J/mol×K	563.39	Joback Method
cpg	295.95	J/mol×K	535.04	Joback Method
cpg	284.97	J/mol×K	506.69	Joback Method

cpg	335.20	J/mol×K	648.44	Joback Method
dvisc	0.0001379	Pa×s	478.34	Joback Method
dvisc	0.0002455	Pa×s	435.39	Joback Method
dvisc	0.0004958	Pa×s	392.45	Joback Method
dvisc	0.0011905	Pa×s	349.50	Joback Method
dvisc	0.0036535	Pa×s	306.55	Joback Method
dvisc	0.0161573	Pa×s	263.61	Joback Method
dvisc	0.1274533	Pa×s	220.66	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=C76649144&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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