

S-(+)-1-Octen-3-ol

Inchi:	InChI=1S/C8H16O/c1-3-5-6-7-8(9)4-2/h4,8-9H,2-3,5-7H2,1H3/t8-/m0/s1
InchiKey:	VSMOENVRRABVKN-QMMMGPBSA-N
Formula:	C8H16O
SMILES:	C=CC(O)CCCC
Mol. weight [g/mol]:	128.21

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
mvol	125.150	ml/mol	McGowan Method
pc	2940.89	kPa	Joback Method
rinpol	962.00		NIST Webbook
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tb	470.86	K	Joback Method
tc	636.76	K	Joback Method
tf	223.98	K	Joback Method
vc	0.477	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	273.08	J/molxK	470.86	Joback Method
cpg	284.36	J/molxK	498.51	Joback Method
cpg	295.19	J/molxK	526.16	Joback Method
cpg	305.56	J/molxK	553.81	Joback Method
cpg	315.50	J/molxK	581.46	Joback Method
cpg	325.02	J/molxK	609.11	Joback Method
cpg	334.14	J/molxK	636.76	Joback Method
dvisc	0.1097275	Paxs	223.98	Joback Method

dvisc	0.0162547	Paxs	265.13	Joback Method
dvisc	0.0040223	Paxs	306.27	Joback Method
dvisc	0.0013856	Paxs	347.42	Joback Method
dvisc	0.0005982	Paxs	388.57	Joback Method
dvisc	0.0003033	Paxs	429.71	Joback Method
dvisc	0.0001732	Paxs	470.86	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R439835&Units=SI

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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