

2,6-Octadien-1-ol

Inchi:	InChI=1S/C8H14O/c1-2-3-4-5-6-7-8-9/h2-3,6-7,9H,4-5,8H2,1H3/b3-2+,7-6+
InchiKey:	ONYJRUXYOCZIAW-BLWKUPHCSA-N
Formula:	C8H14O
SMILES:	CC=CCCC=CCO
Mol. weight [g/mol]:	126.20

Physical Properties

Property code	Value	Unit	Source
gf	40.10	kJ/mol	Joback Method
hf	-126.24	kJ/mol	Joback Method
hfus	20.97	kJ/mol	Joback Method
hvap	50.00	kJ/mol	Joback Method
log10ws	-2.14		Crippen Method
logp	1.891		Crippen Method
mcvol	120.850	ml/mol	McGowan Method
pc	3121.00	kPa	Joback Method
ripol	1232.00		NIST Webbook
ripol	1758.00		NIST Webbook
ripol	1758.00		NIST Webbook
ripol	1758.00		NIST Webbook
tb	482.94	K	Joback Method
tc	657.05	K	Joback Method
tf	230.58	K	Joback Method
vc	0.463	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	256.27	J/molxK	482.94	Joback Method
cpg	305.08	J/molxK	628.03	Joback Method
cpg	296.28	J/molxK	599.01	Joback Method
cpg	287.03	J/molxK	570.00	Joback Method
cpg	277.30	J/molxK	540.98	Joback Method
cpg	267.05	J/molxK	511.96	Joback Method

cpg	313.44	J/molxK	657.05	Joback Method
dvisc	0.0001185	Paxs	482.94	Joback Method
dvisc	0.0002035	Paxs	440.88	Joback Method
dvisc	0.0003915	Paxs	398.82	Joback Method
dvisc	0.0008790	Paxs	356.76	Joback Method
dvisc	0.0024496	Paxs	314.70	Joback Method
dvisc	0.0093657	Paxs	272.64	Joback Method
dvisc	0.0584069	Paxs	230.58	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R507834&Units=SI
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

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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