3,5-Octadien-2-ol

Other names: (E,E)-3,5-Octadien-2-ol
Inchi: InChI=1S/C8H14O/c1-3-4-5-6-7-8(2)9/h4-9H,3H2,1-2H3/b5-4+,7-6+
InchiKey: RQQKJGCMOJSSOV-YTXTXJHMSA-N
Formula: C8H14O
SMILES: CCC=CC=CC(C)O
Mol. weight [g/mol]: 126.20
CAS: 69668-82-2

Physical Properties

Property code	Value	Unit	Source
gf	37.66	kJ/mol	Joback Method
hf	-131.52	kJ/mol	Joback Method
hfus	17.45	kJ/mol	Joback Method
hvap	49.61	kJ/mol	Joback Method
log10ws	-2.25		Crippen Method
logp	1.890		Crippen Method
mcvol	120.850	ml/mol	McGowan Method
pc	3149.09	kPa	Joback Method
rinpol	1039.00		NIST Webbook
rinpol	1038.00		NIST Webbook
rinpol	1037.00		NIST Webbook
tb	482.50	K	Joback Method
tc	660.25	K	Joback Method
tf	215.58	K	Joback Method
vc	0.457	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	256.48	J/mol×K	482.50	Joback Method
cpg	306.50	J/mol×K	630.63	Joback Method
cpg	297.51	J/mol×K	601.00	Joback Method
cpg	288.05	J/mol×K	571.38	Joback Method
cpg	278.07	J/mol×K	541.75	Joback Method

cpg	267.56	J/mol×K	512.13	Joback Method
cpg	315.03	J/mol×K	660.25	Joback Method
dvisc	0.0001127	Pa×s	482.50	Joback Method
dvisc	0.0002021	Pa×s	438.01	Joback Method
dvisc	0.0004134	Pa×s	393.53	Joback Method
dvisc	0.0010151	Pa×s	349.04	Joback Method
dvisc	0.0032406	Pa×s	304.55	Joback Method
dvisc	0.0153884	Pa×s	260.07	Joback Method
dvisc	0.1389924	Pa×s	215.58	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=C69668822&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