

6-Heptene-2,4-diol

Other names:	6-Hepten-2,4-diol
Inchi:	InChI=1S/C7H14O2/c1-3-4-7(9)5-6(2)8/h3,6-9H,1,4-5H2,2H3
InchiKey:	IKSZUZSICAXOHV-UHFFFAOYSA-N
Formula:	C7H14O2
SMILES:	C=CCC(O)CC(C)O
Mol. weight [g/mol]:	130.18
CAS:	19781-76-1

Physical Properties

Property code	Value	Unit	Source
gf	-182.62	kJ/mol	Joback Method
hf	-377.40	kJ/mol	Joback Method
hfus	13.74	kJ/mol	Joback Method
hvap	63.09	kJ/mol	Joback Method
log10ws	-1.36		Crippen Method
logp	0.694		Crippen Method
mcvol	116.930	ml/mol	McGowan Method
pc	3682.02	kPa	Joback Method
rinpol	927.00		NIST Webbook
rinpol	927.00		NIST Webbook
tb	539.72	K	Joback Method
tc	704.59	K	Joback Method
tf	258.53	K	Joback Method
vc	0.434	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	280.76	J/molxK	539.72	Joback Method
cpg	289.91	J/molxK	567.20	Joback Method
cpg	298.67	J/molxK	594.68	Joback Method
cpg	307.04	J/molxK	622.16	Joback Method
cpg	315.04	J/molxK	649.64	Joback Method
cpg	322.68	J/molxK	677.12	Joback Method

cpg	329.98	J/mol×K	704.59	Joback Method
dvisc	0.4158697	Paxs	258.53	Joback Method
dvisc	0.0301816	Paxs	305.39	Joback Method
dvisc	0.0044020	Paxs	352.26	Joback Method
dvisc	0.0010090	Paxs	399.12	Joback Method
dvisc	0.0003152	Paxs	445.99	Joback Method
dvisc	0.0001229	Paxs	492.86	Joback Method
dvisc	0.0000564	Paxs	539.72	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=C19781761&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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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