

6-Methylheptane-1,6-diol

Other names:	6-methyl-1,6-heptanediol
Inchi:	InChI=1S/C8H18O2/c1-8(2,10)6-4-3-5-7-9/h9-10H,3-7H2,1-2H3
InchiKey:	XICLOMYOBVKLTR-UHFFFAOYSA-N
Formula:	C8H18O2
SMILES:	CC(C)(O)CCCCCO
Mol. weight [g/mol]:	146.23
CAS:	5392-57-4

Physical Properties

Property code	Value	Unit	Source
gf	-254.32	kJ/mol	Joback Method
hf	-521.66	kJ/mol	Joback Method
hfus	17.24	kJ/mol	Joback Method
hvap	65.46	kJ/mol	Joback Method
log10ws	-1.81		Crippen Method
logp	1.310		Crippen Method
mcvol	135.320	ml/mol	McGowan Method
pc	3145.56	kPa	Joback Method
tb	563.57	K	Joback Method
tc	727.35	K	Joback Method
tf	303.98	K	Joback Method
vc	0.510	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	348.29	J/molxK	563.57	Joback Method
cpg	358.93	J/molxK	590.87	Joback Method
cpg	369.07	J/molxK	618.16	Joback Method
cpg	378.74	J/molxK	645.46	Joback Method
cpg	387.95	J/molxK	672.76	Joback Method
cpg	396.73	J/molxK	700.06	Joback Method
cpg	405.10	J/molxK	727.35	Joback Method
dvisc	0.0577073	Paxs	303.98	Joback Method

dvisc	0.0082577	Paxs	347.25	Joback Method
dvisc	0.0018180	Paxs	390.51	Joback Method
dvisc	0.0005413	Paxs	433.77	Joback Method
dvisc	0.0002008	Paxs	477.04	Joback Method
dvisc	0.0000878	Paxs	520.30	Joback Method
dvisc	0.0000436	Paxs	563.57	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=C5392574&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀w_s:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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