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

Physical Properties

Property code	Value	Unit	Source
af	0.8010		Cheméo Relay (1.0)
gf	-254.32	kJ/mol	Joback Method
hf	-546.36	kJ/mol	Cheméo Relay (1.0)
hfus	17.24	kJ/mol	Joback Method
hvap	89.60	kJ/mol	Cheméo Relay (1.0)
ie	9.74	eV	Cheméo Relay (1.0)
log10ws	-0.73		Cheméo Relay (1.0)
logp	1.310		Crippen Method
mcvol	135.320	ml/mol	McGowan Method
pc	3145.56	kPa	Joback Method
tb	514.92	K	Cheméo Relay (1.0)
tc	701.93	K	Cheméo Relay (1.0)
tf	311.15	K	Cheméo Relay (1.0)
vc	0.503	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

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

dvisc	0.0005413	Pa×s	433.77	Joback Method
dvisc	0.0000436	Pa×s	563.57	Joback Method
dvisc	0.0000878	Pa×s	520.30	Joback Method
dvisc	0.0002008	Pa×s	477.04	Joback Method
dvisc	0.0577073	Pa×s	303.98	Joback Method
dvisc	0.0018180	Pa×s	390.51	Joback Method
dvisc	0.0082577	Pa×s	347.25	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5392574&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	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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