(S)-(+)-6-METHYL-1-OCTANOL

Other names: d-6-methyl-1-octanol
Inchi: InChI=1S/C9H20O/c1-3-9(2)7-5-4-6-8-10/h9-10H,3-8H2,1-2H3/t9-/m0/s1
InchiKey: WWRGKAMABZHMCN-SECBINFHSA-N
Formula: C9H20O
SMILES: CC[C@H](C)CCCCCO
Mol. weight [g/mol]: 144.26

Physical Properties

Property code	Value	Unit	Source
af	0.6772		Cheméo Relay (1.0)
gf	-114.36	kJ/mol	Joback Method
hf	-404.42	kJ/mol	Cheméo Relay (1.0)
hfus	19.63	kJ/mol	Joback Method
hvap	67.60	kJ/mol	Cheméo Relay (1.0)
ie	9.84	eV	Cheméo Relay (1.0)
log10ws	-2.87		Cheméo Relay (1.0)
logp	2.585		Crippen Method
mcvol	143.540	ml/mol	McGowan Method
pc	2545.61	kPa	Joback Method
tb	483.75	K	Cheméo Relay (1.0)
tc	667.53	K	Cheméo Relay (1.0)
tf	229.84	K	Cheméo Relay (1.0)
vc	0.529	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	334.58	J/mol×K	497.06	Joback Method
cpg	347.30	J/mol×K	524.07	Joback Method
cpg	359.54	J/mol×K	551.09	Joback Method
cpg	371.30	J/mol×K	578.10	Joback Method
cpg	382.60	J/mol×K	605.11	Joback Method
cpg	393.45	J/mol×K	632.13	Joback Method
cpg	403.87	J/mol×K	659.14	Joback Method

dvisc	0.0878509	Pa×s	237.01	Joback Method
dvisc	0.0131188	Pa×s	280.35	Joback Method
dvisc	0.0032599	Pa×s	323.69	Joback Method
dvisc	0.0011254	Pa×s	367.03	Joback Method
dvisc	0.0004864	Pa×s	410.38	Joback Method
dvisc	0.0002468	Pa×s	453.72	Joback Method
dvisc	0.0001409	Pa×s	497.06	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=C110453786&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