3-Heptanol, 2,4-dimethyl-

Other names: 2,4-Dimethyl-3-heptanol
Inchi: InChI=1S/C9H20O/c1-5-6-8(4)9(10)7(2)3/h7-10H,5-6H2,1-4H3
InchiKey: PSCLFHNWSAXNJL-UHFFFAOYSA-N
Formula: C9H20O
SMILES: CCCC(C)C(O)C(C)C
Mol. weight [g/mol]: 144.25
CAS: 19549-72-5

Physical Properties

Property code	Value	Unit	Source
gf	-119.24	kJ/mol	Joback Method
hf	-397.16	kJ/mol	Joback Method
hfus	12.58	kJ/mol	Joback Method
hvap	51.14	kJ/mol	Joback Method
log10ws	-2.48		Crippen Method
logp	2.440		Crippen Method
mcvol	143.540	ml/mol	McGowan Method
pc	2587.22	kPa	Joback Method
ripol	1363.00		NIST Webbook
tb	496.18	K	Joback Method
tc	664.60	K	Joback Method
tf	207.01	K	Joback Method
vc	0.540	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	334.97	J/mol×K	496.18	Joback Method
cpg	348.32	J/mol×K	524.25	Joback Method
cpg	361.14	J/mol×K	552.32	Joback Method
cpg	373.44	J/mol×K	580.39	Joback Method
cpg	385.22	J/mol×K	608.46	Joback Method
cpg	396.50	J/mol×K	636.53	Joback Method
cpg	407.30	J/mol×K	664.60	Joback Method

dvisc	0.5757064	Pa×s	207.01	Joback Method
dvisc	0.0376026	Pa×s	255.20	Joback Method
dvisc	0.0058439	Pa×s	303.40	Joback Method
dvisc	0.0015130	Pa×s	351.59	Joback Method
dvisc	0.0005426	Pa×s	399.79	Joback Method
dvisc	0.0002426	Pa×s	447.98	Joback Method
dvisc	0.0001269	Pa×s	496.18	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19549725&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume