1-Octanol, 2,7-dimethyl-

Other names: 2,7-dimethyl-1-octanol
Inchi: InChI=1S/C10H22O/c1-9(2)6-4-5-7-10(3)8-11/h9-11H,4-8H2,1-3H3
InchiKey: FNLOIWOIWFHQSI-UHFFFAOYSA-N
Formula: C10H22O
SMILES: CC(C)CCCCC(C)CO
Mol. weight [g/mol]: 158.28
CAS: 15250-22-3

Physical Properties

Property code	Value	Unit	Source
gf	-108.38	kJ/mol	Joback Method
hf	-412.52	kJ/mol	Joback Method
hfus	18.70	kJ/mol	Joback Method
hvap	53.76	kJ/mol	Joback Method
log10ws	-2.79		Crippen Method
logp	2.831		Crippen Method
mcvol	157.630	ml/mol	McGowan Method
pc	2333.78	kPa	Joback Method
rinpol	144.10		NIST Webbook
ripol	1625.00		NIST Webbook
tb	519.50	K	Joback Method
tc	683.75	K	Joback Method
tf	233.28	K	Joback Method
vc	0.603	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	381.07	J/mol×K	519.50	Joback Method
cpg	394.90	J/mol×K	546.87	Joback Method
cpg	408.18	J/mol×K	574.25	Joback Method
cpg	420.93	J/mol×K	601.62	Joback Method
cpg	433.16	J/mol×K	629.00	Joback Method
cpg	444.88	J/mol×K	656.37	Joback Method

cpg	456.11	J/mol×K	683.75	Joback Method
dvisc	0.1480969	Pa×s	233.28	Joback Method
dvisc	0.0161218	Pa×s	280.98	Joback Method
dvisc	0.0033408	Pa×s	328.69	Joback Method
dvisc	0.0010317	Pa×s	376.39	Joback Method
dvisc	0.0004150	Pa×s	424.09	Joback Method
dvisc	0.0002007	Pa×s	471.80	Joback Method
dvisc	0.0001109	Pa×s	519.50	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=C15250223&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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