3-Pentanol, 2,2,4,4-tetramethyl-

Other names: 2,2,4,4-Tetramethylpentan-3-ol
Inchi: InChI=1S/C9H20O/c1-8(2,3)7(10)9(4,5)6/h7,10H,1-6H3
InchiKey: WFJSIIHYYLHRHB-UHFFFAOYSA-N
Formula: C9H20O
SMILES: CC(C)(C)C(O)C(C)(C)C
Mol. weight [g/mol]: 144.25
CAS: 14609-79-1

Physical Properties

Property code	Value	Unit	Source
gf	-108.68	kJ/mol	Joback Method
hf	-404.10	kJ/mol	Joback Method
hfus	4.80	kJ/mol	Joback Method
hvap	62.70 ± 0.90	kJ/mol	NIST Webbook
log10ws	-2.48		Crippen Method
logp	2.440		Crippen Method
mcvol	143.540	ml/mol	McGowan Method
pc	2646.11	kPa	Joback Method
tb	442.65 ± 4.00	K	NIST Webbook
tb	437.65 ± 3.00	K	NIST Webbook
tb	438.65 ± 4.00	K	NIST Webbook
tb	437.15 ± 5.00	K	NIST Webbook
tb	439.15 ± 4.00	K	NIST Webbook
tb	439.00 ± 5.00	K	NIST Webbook
tb	438.65 ± 4.00	K	NIST Webbook
tc	671.71	K	Joback Method
tf	320.15 ± 2.00	K	NIST Webbook
tf	325.00 ± 3.00	K	NIST Webbook
tf	325.00 ± 3.00	K	NIST Webbook
vc	0.530	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	417.23	J/mol×K	671.71	Joback Method
cpg	406.20	J/mol×K	641.53	Joback Method
cpg	394.50	J/mol×K	611.34	Joback Method
cpg	382.10	J/mol×K	581.16	Joback Method
cpg	368.96	J/mol×K	550.97	Joback Method
cpg	355.03	J/mol×K	520.79	Joback Method
cpg	340.27	J/mol×K	490.60	Joback Method
dvisc	0.1725436	Pa×s	241.85	Joback Method
dvisc	0.0001395	Pa×s	490.60	Joback Method
dvisc	0.0002643	Pa×s	449.14	Joback Method
dvisc	0.0005702	Pa×s	407.68	Joback Method
dvisc	0.0014643	Pa×s	366.23	Joback Method
dvisc	0.0047838	Pa×s	324.77	Joback Method
dvisc	0.0221006	Pa×s	283.31	Joback Method
hfust	7.30	kJ/mol	322.00	NIST Webbook

Sources

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=C14609791&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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
hfust: Enthalpy of fusion at a given temperature
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
tb: Normal Boiling Point Temperature

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume