3-Pentanol, 3-(1,1-dimethylethyl)-2,2,4,4-tetramethyl-

Inchi: InChI=1S/C13H28O/c1-10(2,3)13(14,11(4,5)6)12(7,8)9/h14H,1-9H3
InchiKey: LIUBOLYWYDGCSJ-UHFFFAOYSA-N
Formula: C13H28O
SMILES: CC(C)(C)C(O)(C(C)(C)C)C(C)(C)C
Mol. weight [g/mol]: 200.36
CAS: 41902-42-5

Physical Properties

Property code	Value	Unit	Source
chs	-8643.90 ± 3.80	kJ/mol	NIST Webbook
gf	-66.88	kJ/mol	Joback Method
hf	-410.10 ± 4.00	kJ/mol	NIST Webbook
hfs	-473.30 ± 3.80	kJ/mol	NIST Webbook
hfus	3.86	kJ/mol	Joback Method
hsub	63.20 ± 1.20	kJ/mol	NIST Webbook
hsub	63.20	kJ/mol	NIST Webbook
hvap	56.03	kJ/mol	Joback Method
log10ws	-3.91		Crippen Method
logp	3.856		Crippen Method
mcvol	199.900	ml/mol	McGowan Method
pc	1893.65	kPa	Joback Method
tb	576.10	K	Joback Method
tc	766.16	K	Joback Method
tf	368.00 ± 2.00	K	NIST Webbook
tf	390.15 ± 0.02	K	NIST Webbook
vc	0.739	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	621.95	J/mol×K	734.48	Joback Method
cpg	607.83	J/mol×K	702.81	Joback Method
cpg	592.76	J/mol×K	671.13	Joback Method
cpg	576.67	J/mol×K	639.45	Joback Method

cpg	559.46	J/mol×K	607.78	Joback Method
cpg	541.05	J/mol×K	576.10	Joback Method
cpg	635.21	J/mol×K	766.16	Joback Method
cps	350.60	J/mol×K	298.15	NIST Webbook
dvisc	0.0314996	Pa×s	306.77	Joback Method
dvisc	0.0000510	Pa×s	576.10	Joback Method
dvisc	0.0000947	Pa×s	531.21	Joback Method
dvisc	0.0001970	Pa×s	486.32	Joback Method
dvisc	0.0004758	Pa×s	441.43	Joback Method
dvisc	0.0014027	Pa×s	396.55	Joback Method
dvisc	0.0054498	Pa×s	351.66	Joback Method
hfust	3.43	kJ/mol	390.00	NIST Webbook
hfust	3.43	kJ/mol	390.15	NIST Webbook
sfust	8.80	J/mol×K	390.15	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C41902425&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

Legend

chs: Standard solid enthalpy of combustion
cpg: Ideal gas heat capacity
cps: Solid phase heat capacity
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfs: Solid phase enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hfust: Enthalpy of fusion at a given temperature
hsub: Enthalpy of sublimation 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
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume