2,2,4-Trimethyl-3-pentanol

Other names: 2,2,4-trimethylpentan-3-ol
3-Pentanol, 2,2,4-trimethyl-
Inchi: InChI=1S/C8H18O/c1-6(2)7(9)8(3,4)5/h6-7,9H,1-5H3
InchiKey: AXINNNJHLJWMTC-UHFFFAOYSA-N
Formula: C8H18O
SMILES: CC(C)C(O)C(C)(C)C
Mol. weight [g/mol]: 130.23
CAS: 5162-48-1

Physical Properties

Property code	Value	Unit	Source
gf	-122.38	kJ/mol	Joback Method
hf	-379.99	kJ/mol	Joback Method
hfus	6.10	kJ/mol	Joback Method
hvap	48.01	kJ/mol	Joback Method
log10ws	-2.06		Crippen Method
logp	2.049		Crippen Method
mcvol	129.450	ml/mol	McGowan Method
pc	2893.62	kPa	Joback Method
rinpol	882.00		NIST Webbook
rinpol	882.00		NIST Webbook
tb	423.15 ± 3.00	K	NIST Webbook
tb	423.15 ± 3.00	K	NIST Webbook
tb	418.15 ± 6.00	K	NIST Webbook
tb	418.15 ± 2.00	K	NIST Webbook
tb	419.65 ± 3.00	K	NIST Webbook
tb	423.65 ± 3.00	K	NIST Webbook
tb	418.15 ± 5.00	K	NIST Webbook
tb	426.15 ± 3.00	K	NIST Webbook
tb	428.15 ± 2.00	K	NIST Webbook
tb	424.45 ± 1.00	K	NIST Webbook
tb	422.15 ± 3.00	K	NIST Webbook
tb	424.15 ± 1.00	K	NIST Webbook
tb	420.15 ± 2.00	K	NIST Webbook
tb	423.65 ± 3.00	K	NIST Webbook
tc	646.51	K	Joback Method
tf	213.16	K	Joback Method

vc	0.479	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	293.13	J/mol×K	470.51	Joback Method
cpg	306.34	J/mol×K	499.84	Joback Method
cpg	318.90	J/mol×K	529.18	Joback Method
cpg	330.85	J/mol×K	558.51	Joback Method
cpg	342.21	J/mol×K	587.85	Joback Method
cpg	353.00	J/mol×K	617.18	Joback Method
cpg	363.24	J/mol×K	646.51	Joback Method
dvisc	0.4662578	Pa×s	213.16	Joback Method
dvisc	0.0408132	Pa×s	256.05	Joback Method
dvisc	0.0071866	Pa×s	298.94	Joback Method
dvisc	0.0019567	Pa×s	341.84	Joback Method
dvisc	0.0007121	Pa×s	384.73	Joback Method
dvisc	0.0003174	Pa×s	427.62	Joback Method
dvisc	0.0001639	Pa×s	470.51	Joback Method
hvapt	57.10	kJ/mol	378.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.39970e+01
Coeff. B	-2.55387e+03
Coeff. C	-1.49693e+02
Temperature range (K), min.	335.98
Temperature range (K), max.	443.73

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=C5162481&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume