

2,4,4-Trimethyl-1-pentanol

Other names:	1-Pentanol, 2,4,4-trimethyl- 2,4,4-trimethylpentan-1-ol
Inchi:	InChI=1S/C8H18O/c1-7(6-9)5-8(2,3)4/h7,9H,5-6H2,1-4H3
InchiKey:	ZNRVRWHPZZOTIE-UHFFFAOYSA-N
Formula:	C8H18O
SMILES:	CC(CO)CC(C)(C)C
Mol. weight [g/mol]:	130.23
CAS:	16325-63-6

Physical Properties

Property code	Value	Unit	Source
gf	-119.94	kJ/mol	Joback Method
hf	-374.71	kJ/mol	Joback Method
hfus	9.63	kJ/mol	Joback Method
hvap	48.40	kJ/mol	Joback Method
log10ws	-1.95		Crippen Method
logp	2.051		Crippen Method
mcvol	129.450	ml/mol	McGowan Method
pc	2868.87	kPa	Joback Method
tb	443.65 ± 3.00	K	NIST Webbook
tc	643.32	K	Joback Method
tf	228.16	K	Joback Method
vc	0.485	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	292.99	J/mol×K	470.95	Joback Method
cpg	305.85	J/mol×K	499.68	Joback Method
cpg	318.10	J/mol×K	528.41	Joback Method
cpg	329.77	J/mol×K	557.13	Joback Method
cpg	340.87	J/mol×K	585.86	Joback Method
cpg	351.43	J/mol×K	614.59	Joback Method
cpg	361.48	J/mol×K	643.32	Joback Method

dvisc	0.1736472	Paxs	228.16	Joback Method
dvisc	0.0230030	Paxs	268.62	Joback Method
dvisc	0.0051732	Paxs	309.09	Joback Method
dvisc	0.0016435	Paxs	349.55	Joback Method
dvisc	0.0006624	Paxs	390.02	Joback Method
dvisc	0.0003167	Paxs	430.49	Joback Method
dvisc	0.0001719	Paxs	470.95	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	441.70	K	98.70	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.60182e+01
Coeff. B	-4.43045e+03
Coeff. C	-5.50100e+01
Temperature range (K), min.	336.66
Temperature range (K), max.	468.81

Sources

The Yaws Handbook of Vapor Pressure:
Crippen Method:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>
<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>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C16325636&Units=SI>

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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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