4,4-DIMETHYL-2-PENTANOL

Other names: 4,4-dimethylpentan-2-ol
Methylneopentylcarbinol
Inchi: InChI=1S/C7H16O/c1-6(8)5-7(2,3)4/h6,8H,5H2,1-4H3
InchiKey: OIBKGNPMOMMSSI-UHFFFAOYSA-N
Formula: C7H16O
SMILES: CC(O)CC(C)(C)C
Mol. weight [g/mol]: 116.20
CAS: 6144-93-0

Physical Properties

Property code	Value	Unit	Source
af	0.5330		Cheméo Relay (1.0)
gf	-128.36	kJ/mol	Joback Method
hf	-395.19	kJ/mol	Cheméo Relay (1.0)
hfus	7.04	kJ/mol	Joback Method
hvap	54.71	kJ/mol	Cheméo Relay (1.0)
ie	9.67	eV	Cheméo Relay (1.0)
log10ws	-1.07		Cheméo Relay (1.0)
logp	1.803		Crippen Method
mcvol	115.360	ml/mol	McGowan Method
pc	3188.33	kPa	Joback Method
ripol	1219.90		NIST Webbook
tb	410.65 ± 3.00	K	NIST Webbook
tb	411.15 ± 2.00	K	NIST Webbook
tc	575.96	K	Cheméo Relay (1.0)
tf	244.41	K	Cheméo Relay (1.0)
vc	0.415	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	250.49	J/mol×K	448.07	Joback Method
cpg	313.99	J/mol×K	621.71	Joback Method
cpg	304.69	J/mol×K	592.77	Joback Method

cpg	294.91	J/mol×K	563.83	Joback Method
cpg	284.62	J/mol×K	534.89	Joback Method
cpg	273.81	J/mol×K	505.95	Joback Method
cpg	262.44	J/mol×K	477.01	Joback Method
dvisc	0.0021138	Pa×s	332.48	Joback Method
dvisc	0.0002114	Pa×s	448.07	Joback Method
dvisc	0.0003942	Pa×s	409.54	Joback Method
dvisc	0.0008366	Pa×s	371.01	Joback Method
dvisc	0.2459675	Pa×s	216.89	Joback Method
dvisc	0.0068100	Pa×s	293.95	Joback Method
dvisc	0.0312263	Pa×s	255.42	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	410.50	K	98.10	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.51507e+01
Coeff. B	-3.41435e+03
Coeff. C	-8.64730e+01
Temperature range (K), min.	316.19
Temperature range (K), max.	433.49

Sources

Cheméo Relay (1.0, beta):

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6144930&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	

Legend

af:	Acentric Factor
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume