

1,3,5-PENTANETRIOL

Inchi:	InChI=1S/C5H12O3/c6-3-1-5(8)2-4-7/h5-8H,1-4H2
InchiKey:	LMMTVYUCEFJZLC-UHFFFAOYSA-N
Formula:	C5H12O3
SMILES:	OCCC(O)CCO
Mol. weight [g/mol]:	120.15

Physical Properties

Property code	Value	Unit	Source
hf	-607.11	kJ/mol	Cheméo Relay (1.0)
hfus	17.45	kJ/mol	Joback Method
hvap	100.18	kJ/mol	Cheméo Relay (1.0)
ie	9.87	eV	Cheméo Relay (1.0)
log10ws	0.58		Cheméo Relay (1.0)
logp	-0.888		Crippen Method
mcvol	98.920	ml/mol	McGowan Method
pc	5001.51	kPa	Joback Method
tb	560.67	K	Cheméo Relay (1.0)
tc	779.92	K	Cheméo Relay (1.0)
tf	300.69	K	Cheméo Relay (1.0)
vc	0.367	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	255.26	J/mol×K	589.90	Joback Method
cpg	262.05	J/mol×K	616.27	Joback Method
cpg	268.57	J/mol×K	642.64	Joback Method
cpg	274.82	J/mol×K	669.01	Joback Method
cpg	280.81	J/mol×K	695.38	Joback Method
cpg	286.54	J/mol×K	721.75	Joback Method
cpg	292.03	J/mol×K	748.12	Joback Method
dvisc	0.1188974	Pa×s	313.57	Joback Method
dvisc	0.0103489	Pa×s	359.62	Joback Method
dvisc	0.0015680	Pa×s	405.68	Joback Method

dvisc	0.0003491	Pa×s	451.74	Joback Method
dvisc	0.0001026	Pa×s	497.79	Joback Method
dvisc	0.0000371	Pa×s	543.85	Joback Method
dvisc	0.0000157	Pa×s	589.90	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C4328943&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

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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