

(SS)- or (RR)-4-methyl-2,3-pentandiol

Inchi:	InChI=1S/C6H14O2/c1-4(2)6(8)5(3)7/h4-8H,1-3H3
InchiKey:	RNKURRDNOYXATR-UHFFFAOYSA-N
Formula:	C6H14O2
SMILES:	CC(C)C(O)C(C)O
Mol. weight [g/mol]:	118.17
CAS:	6464-40-0

Physical Properties

Property code	Value	Unit	Source
gf	-281.32	kJ/mol	Joback Method
hf	-487.47	kJ/mol	Joback Method
hfus	8.90	kJ/mol	Joback Method
hvap	61.14	kJ/mol	Joback Method
log10ws	-0.84		Crippen Method
logp	0.384		Crippen Method
mcvol	107.140	ml/mol	McGowan Method
pc	3975.52	kPa	Joback Method
tb	519.72	K	Joback Method
tc	685.78	K	Joback Method
tf	234.02	K	Joback Method
vc	0.392	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	256.00	J/molxK	519.72	Joback Method
cpg	265.09	J/molxK	547.40	Joback Method
cpg	273.80	J/molxK	575.07	Joback Method
cpg	282.15	J/molxK	602.75	Joback Method
cpg	290.15	J/molxK	630.43	Joback Method
cpg	297.80	J/molxK	658.10	Joback Method
cpg	305.12	J/molxK	685.78	Joback Method
dvisc	2.1854148	Paxs	234.02	Joback Method
dvisc	0.0891622	Paxs	281.64	Joback Method

dvisc	0.0091767	Paxs	329.25	Joback Method
dvisc	0.0016777	Paxs	376.87	Joback Method
dvisc	0.0004491	Paxs	424.49	Joback Method
dvisc	0.0001568	Paxs	472.10	Joback Method
dvisc	0.0000664	Paxs	519.72	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6464400&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

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
mccvol:	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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