

(SR)- OR (RS)-4-METHYL-2,3-PENTANEDIOL

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]:

118.18

Physical Properties

Property code	Value	Unit	Source
af	0.6428		Cheméo Relay (1.0)
gf	-281.32	kJ/mol	Joback Method
hf	-482.53	kJ/mol	Cheméo Relay (1.0)
hfus	8.90	kJ/mol	Joback Method
hvap	71.77	kJ/mol	Cheméo Relay (1.0)
ie	9.87	eV	Cheméo Relay (1.0)
log10ws	-0.28		Cheméo Relay (1.0)
logp	0.384		Crippen Method
mcvol	107.140	ml/mol	McGowan Method
pc	3975.52	kPa	Joback Method
tb	460.02	K	Cheméo Relay (1.0)
tc	624.23	K	Cheméo Relay (1.0)
tf	293.73	K	Cheméo Relay (1.0)
vc	0.398	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	256.00	J/mol×K	519.72	Joback Method
cpg	265.09	J/mol×K	547.40	Joback Method
cpg	273.80	J/mol×K	575.07	Joback Method
cpg	282.15	J/mol×K	602.75	Joback Method
cpg	290.15	J/mol×K	630.43	Joback Method
cpg	297.80	J/mol×K	658.10	Joback Method
cpg	305.12	J/mol×K	685.78	Joback Method
dvisc	2.1854148	Pa×s	234.02	Joback Method

dvisc	0.0891622	Pa×s	281.64	Joback Method
dvisc	0.0091767	Pa×s	329.25	Joback Method
dvisc	0.0016777	Pa×s	376.87	Joback Method
dvisc	0.0004491	Pa×s	424.49	Joback Method
dvisc	0.0001568	Pa×s	472.10	Joback Method
dvisc	0.0000664	Pa×s	519.72	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6702109&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):	
Cheméo Relay (1.0, beta):	

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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