(SS)- OR (RR)-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	305.12	J/mol×K	685.78	Joback Method
cpg	297.80	J/mol×K	658.10	Joback Method
cpg	290.15	J/mol×K	630.43	Joback Method
cpg	282.15	J/mol×K	602.75	Joback Method
cpg	273.80	J/mol×K	575.07	Joback Method
cpg	265.09	J/mol×K	547.40	Joback Method
dvisc	0.0016777	Pa×s	376.87	Joback Method

dvisc	0.0000664	Pa×s	519.72	Joback Method
dvisc	0.0001568	Pa×s	472.10	Joback Method
dvisc	0.0004491	Pa×s	424.49	Joback Method
dvisc	2.1854148	Pa×s	234.02	Joback Method
dvisc	0.0091767	Pa×s	329.25	Joback Method
dvisc	0.0891622	Pa×s	281.64	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6464400&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