

1,2,3,4-Butanetetrol, [S-(R*,R*)]-

Other names:	Threitol, L- l-Threitol L-1,2,3,4-Butanetetraol
Inchi:	InChI=1S/C4H10O4/c5-1-3(7)4(8)2-6/h3-8H,1-2H2/t3-,4-/m0/s1
InchiKey:	UNXHWFMMPAWVPI-IMJSIDKUSA-N
Formula:	C4H10O4
SMILES:	OCC(O)C(O)CO
Mol. weight [g/mol]:	122.12
CAS:	2319-57-5

Physical Properties

Property code	Value	Unit	Source
gf	-569.36	kJ/mol	Joback Method
hf	-745.37	kJ/mol	Joback Method
hfus	15.42	kJ/mol	Joback Method
hsub	123.00	kJ/mol	NIST Webbook
hvap	90.44	kJ/mol	Joback Method
log10ws	1.23		Crippen Method
logp	-2.307		Crippen Method
mcvol	90.700	ml/mol	McGowan Method
pc	6740.71	kPa	Joback Method
tb	658.76	K	Joback Method
tc	819.90	K	Joback Method
tf	360.00 ± 5.00	K	NIST Webbook
vc	0.324	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	273.46	J/molxK	793.04	Joback Method
cpg	277.70	J/molxK	819.90	Joback Method
cpg	248.93	J/molxK	658.76	Joback Method
cpg	254.30	J/molxK	685.62	Joback Method
cpg	259.43	J/molxK	712.47	Joback Method

cpg	264.33	J/mol×K	739.33	Joback Method
cpg	269.00	J/mol×K	766.19	Joback Method
dvisc	0.0000022	Paxs	658.76	Joback Method
dvisc	0.0000058	Paxs	606.99	Joback Method
dvisc	0.0672433	Paxs	348.12	Joback Method
dvisc	0.0039218	Paxs	399.89	Joback Method
dvisc	0.0004388	Paxs	451.67	Joback Method
dvisc	0.0000770	Paxs	503.44	Joback Method
dvisc	0.0000187	Paxs	555.21	Joback Method
hfust	29.10	kJ/mol	361.80	NIST Webbook
hvapt	86.00 ± 1.00	kJ/mol	398.00	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2319575&Units=SI

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
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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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