1,2,3-Butanetriol

Other names: butane-1,2,3-triol
Inchi: InChI=1S/C4H10O3/c1-3(6)4(7)2-5/h3-7H,2H2,1H3
InchiKey: YAXKTBLXMTYWDQ-UHFFFAOYSA-N
Formula: C4H10O3
SMILES: CC(O)C(O)CO
Mol. weight [g/mol]: 106.12
CAS: 4435-50-1

Physical Properties

Property code	Value	Unit	Source
gf	-432.54	kJ/mol	Joback Method
hf	-593.14	kJ/mol	Joback Method
hfus	11.33	kJ/mol	Joback Method
hvap	73.76	kJ/mol	Joback Method
log10ws	0.49		Crippen Method
logp	-1.280		Crippen Method
mcvol	84.830	ml/mol	McGowan Method
pc	5827.17	kPa	Joback Method
tb	566.58	K	Joback Method
tc	727.30	K	Joback Method
tf	287.30	K	Joback Method
vc	0.304	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	211.95	J/mol×K	566.58	Joback Method
cpg	217.97	J/mol×K	593.37	Joback Method
cpg	223.75	J/mol×K	620.15	Joback Method
cpg	229.28	J/mol×K	646.94	Joback Method
cpg	234.57	J/mol×K	673.73	Joback Method
cpg	239.63	J/mol×K	700.52	Joback Method
cpg	244.47	J/mol×K	727.30	Joback Method
dvisc	0.5264520	Pa×s	287.30	Joback Method

dvisc	0.0297399	Pa×s	333.85	Joback Method
dvisc	0.0033943	Pa×s	380.39	Joback Method
dvisc	0.0006218	Pa×s	426.94	Joback Method
dvisc	0.0001591	Pa×s	473.49	Joback Method
dvisc	0.0000519	Pa×s	520.03	Joback Method
dvisc	0.0000204	Pa×s	566.58	Joback Method
hvapt	68.10	kJ/mol	456.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4435501&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
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