4-(Methylthio)butanol

Other names:	4-(Methylsulfanyl)-1-butanol
	1-Butanol, 4-methylthio
	4-Methylthiobutan-1-ol
	4-methylsulfanylbutan-1-ol
Inchi:	InChI=1S/C5H12OS/c1-7-5-3-2-4-6/h6H,2-5H2,1H3
InchiKey:	JNTVUHZXIJFHAU-UHFFFAOYSA-N
Formula:	C5H12OS
SMILES:	CSCCCCO
Mol. weight [g/mol]:	120.22

Physical Properties

Property code	Value	Unit	Source
af	0.6127		Cheméo Relay (1.0)
gf	-112.48	kJ/mol	Joback Method
hf	-278.82	kJ/mol	Cheméo Relay (1.0)
hfus	16.92	kJ/mol	Joback Method
hvap	72.80	kJ/mol	Cheméo Relay (1.0)
ie	8.77	eV	Cheméo Relay (1.0)
log10ws	-0.01		Cheméo Relay (1.0)
logp	1.122		Crippen Method
mcvol	103.530	ml/mol	McGowan Method
pc	3960.52	kPa	Joback Method
ripol	1812.00		NIST Webbook
ripol	1812.00		NIST Webbook
tb	488.76	K	Cheméo Relay (1.0)
tc	722.74	K	Cheméo Relay (1.0)
tf	248.04	K	Cheméo Relay (1.0)
vc	0.361	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	213.63	J/mol×K	474.96	Joback Method
cpg	222.60	J/mol×K	505.34	Joback Method

cpg	231.22	J/mol×K	535.71	Joback Method
cpg	239.50	J/mol×K	566.09	Joback Method
cpg	247.42	J/mol×K	596.47	Joback Method
cpg	255.01	J/mol×K	626.84	Joback Method
cpg	262.27	J/mol×K	657.22	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C20582858&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

Legend

af: Acentric Factor
cpg: Ideal gas heat capacity
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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.