

Butane, 1-(ethylsulfinyl)-

Other names:	Sulfoxide, butyl ethyl Butyl ethyl sulfoxide Ethyl-n-butylsulfoxide
Inchi:	InChI=1S/C6H14OS/c1-3-5-6-8(7)4-2/h3-6H2,1-2H3
InchiKey:	CYDQHOZLSSXJKU-UHFFFAOYSA-N
Formula:	C6H14OS
SMILES:	CCCCS(=O)CC
Mol. weight [g/mol]:	134.24
CAS:	2976-99-0

Physical Properties

Property code	Value	Unit	Source
gf	-218.07	kJ/mol	Joback Method
hf	-372.91	kJ/mol	Joback Method
hfus	19.05	kJ/mol	Joback Method
hvap	41.68	kJ/mol	Joback Method
log10ws	-0.97		Crippen Method
logp	1.555		Crippen Method
mcvol	117.620	ml/mol	McGowan Method
pc	3427.87	kPa	Joback Method
tb	394.96	K	Joback Method
tc	570.30	K	Joback Method
tf	193.86	K	Joback Method
vc	0.462	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	217.98	J/mol×K	394.96	Joback Method
cpg	229.40	J/mol×K	424.18	Joback Method
cpg	240.43	J/mol×K	453.41	Joback Method
cpg	251.06	J/mol×K	482.63	Joback Method
cpg	261.30	J/mol×K	511.85	Joback Method
cpg	271.16	J/mol×K	541.08	Joback Method

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=C2976990&Units=SI

Legend

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	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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