Butane, 1-(ethylsulfonyl)-

Other names:	Sulfone, butyl ethyl
	Butyl ethyl sulfone
Inchi:	InChI=1S/C6H14O2S/c1-3-5-6-9(7,8)4-2/h3-6H2,1-2H3
InchiKey:	PVSJGAIWOIMZFG-UHFFFAOYSA-N
Formula:	C6H14O2S
SMILES:	CCCCS(=O)(=O)CC
Mol. weight [g/mol]:	150.24
CAS:	31124-38-6

Physical Properties

Property code	Value	Unit	Source
gf	-468.90	kJ/mol	Joback Method
hf	-620.52	kJ/mol	Joback Method
hfus	22.67	kJ/mol	Joback Method
hvap	47.58	kJ/mol	Joback Method
log10ws	-1.17		Crippen Method
logp	1.221		Crippen Method
mcvol	123.490	ml/mol	McGowan Method
pc	3722.56	kPa	Joback Method
tb	384.46	K	Joback Method
tc	547.33	K	Joback Method
tf	357.00 ± 2.00	K	NIST Webbook
tf	323.00 ± 4.00	K	NIST Webbook
tf	321.00 ± 4.00	K	NIST Webbook
tf	322.20 ± 0.50	K	NIST Webbook
tf	324.00 ± 5.00	K	NIST Webbook
vc	0.497	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	229.01	J/mol×K	384.46	Joback Method
cpg	240.33	J/mol×K	411.61	Joback Method
cpg	251.31	J/mol×K	438.75	Joback Method

cpg	261.93	J/mol×K	465.90	Joback Method
cpg	272.19	J/mol×K	493.04	Joback Method
cpg	282.10	J/mol×K	520.19	Joback Method
cpg	291.65	J/mol×K	547.33	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C31124386&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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume