

sec-Butyl ethyl sulphoxide

Inchi:	InChI=1S/C6H14OS/c1-4-6(3)8(7)5-2/h6H,4-5H2,1-3H3
InchiKey:	LEWXGMHZJYIGGE-UHFFFAOYSA-N
Formula:	C6H14OS
SMILES:	CCC(C)S(=O)CC
Mol. weight [g/mol]:	134.24

Physical Properties

Property code	Value	Unit	Source
hfus	15.53	kJ/mol	Joback Method
logp	1.554		Crippen Method
mcvol	117.620	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	217.93	J/mol×K	394.52	Joback Method
cpg	229.71	J/mol×K	424.43	Joback Method
cpg	241.07	J/mol×K	454.34	Joback Method
cpg	252.01	J/mol×K	484.25	Joback Method
cpg	262.54	J/mol×K	514.15	Joback Method
cpg	272.65	J/mol×K	544.06	Joback Method
cpg	282.36	J/mol×K	573.97	Joback Method

Sources

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
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7694180&Units=SI

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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<https://www.chemeo.com/cid/45-082-1/sec-Butyl-ethyl-sulphoxide.pdf>

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