2-[Butylthio]ethanal

Inchi: InChI=1S/C6H12OS/c1-2-3-5-8-6-4-7/h4H,2-3,5-6H2,1H3
InchiKey: WZLVGITZGOFMOU-UHFFFAOYSA-N
Formula: C6H12OS
SMILES: CCCCSCC=O
Mol. weight [g/mol]: 132.22

Physical Properties

Property code	Value	Unit	Source
gf	-66.76	kJ/mol	Joback Method
hf	-210.88	kJ/mol	Joback Method
hfus	17.71	kJ/mol	Joback Method
hvap	42.49	kJ/mol	Joback Method
log10ws	-1.50		Crippen Method
logp	1.719		Crippen Method
mcvol	113.320	ml/mol	McGowan Method
pc	3448.03	kPa	Joback Method
ripol	1564.00		NIST Webbook
ripol	1564.00		NIST Webbook
tb	454.12	K	Joback Method
tc	649.52	K	Joback Method
tf	233.78	K	Joback Method
vc	0.443	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	225.08	J/mol×K	454.12	Joback Method
cpg	235.58	J/mol×K	486.69	Joback Method
cpg	245.65	J/mol×K	519.25	Joback Method
cpg	255.27	J/mol×K	551.82	Joback Method
cpg	264.45	J/mol×K	584.39	Joback Method
cpg	273.21	J/mol×K	616.96	Joback Method
cpg	281.55	J/mol×K	649.52	Joback Method

Sources

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=R402105&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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