2-[Isobutylthio]ethanal

Inchi: InChI=1S/C6H12OS/c1-6(2)5-8-4-3-7/h3,6H,4-5H2,1-2H3
InchiKey: GAJKCQHEVMCMEJ-UHFFFAOYSA-N
Formula: C6H12OS
SMILES: CC(C)CSCC=O
Mol. weight [g/mol]: 132.22

Physical Properties

Property code	Value	Unit	Source
gf	-69.20	kJ/mol	Joback Method
hf	-216.16	kJ/mol	Joback Method
hfus	14.19	kJ/mol	Joback Method
hvap	42.10	kJ/mol	Joback Method
log10ws	-1.26		Crippen Method
logp	1.575		Crippen Method
mcvol	113.320	ml/mol	McGowan Method
pc	3480.65	kPa	Joback Method
ripol	1479.00		NIST Webbook
ripol	1479.00		NIST Webbook
tb	453.68	K	Joback Method
tc	653.63	K	Joback Method
tf	218.78	K	Joback Method
vc	0.436	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	225.23	J/mol×K	453.68	Joback Method
cpg	236.07	J/mol×K	487.00	Joback Method
cpg	246.43	J/mol×K	520.33	Joback Method
cpg	256.33	J/mol×K	553.65	Joback Method
cpg	265.75	J/mol×K	586.98	Joback Method
cpg	274.73	J/mol×K	620.30	Joback Method
cpg	283.25	J/mol×K	653.63	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R402130&Units=SI
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

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