2-[But-2-enylthio]ethanal

Inchi: InChI=1S/C6H10OS/c1-2-3-5-8-6-4-7/h2-4H,5-6H2,1H3/b3-2+
InchiKey: ONEQLHKTAKJQBB-NSCUHMNNSA-N
Formula: C6H10OS
SMILES: CC=CCSCC=O
Mol. weight [g/mol]: 130.21

Physical Properties

Property code	Value	Unit	Source
gf	13.46	kJ/mol	Joback Method
hf	-93.66	kJ/mol	Joback Method
hfus	17.92	kJ/mol	Joback Method
hvap	42.45	kJ/mol	Joback Method
log10ws	-1.35		Crippen Method
logp	1.495		Crippen Method
mcvol	109.020	ml/mol	McGowan Method
pc	3668.65	kPa	Joback Method
ripol	1605.00		NIST Webbook
ripol	1605.00		NIST Webbook
tb	458.28	K	Joback Method
tc	663.42	K	Joback Method
tf	228.70	K	Joback Method
vc	0.422	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	208.39	J/mol×K	458.28	Joback Method
cpg	218.41	J/mol×K	492.47	Joback Method
cpg	227.90	J/mol×K	526.66	Joback Method
cpg	236.89	J/mol×K	560.85	Joback Method
cpg	245.40	J/mol×K	595.04	Joback Method
cpg	253.43	J/mol×K	629.23	Joback Method
cpg	261.02	J/mol×K	663.42	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=R402081&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume