2-[Propylthio]ethanal

Inchi: InChI=1S/C5H10OS/c1-2-4-7-5-3-6/h3H,2,4-5H2,1H3
InchiKey: CJGGFVSOYXYNTR-UHFFFAOYSA-N
Formula: C5H10OS
SMILES: CCCSCC=O
Mol. weight [g/mol]: 118.20

Physical Properties

Property code	Value	Unit	Source
gf	-75.18	kJ/mol	Joback Method
hf	-190.24	kJ/mol	Joback Method
hfus	15.12	kJ/mol	Joback Method
hvap	40.26	kJ/mol	Joback Method
log10ws	-1.08		Crippen Method
logp	1.329		Crippen Method
mcvol	99.230	ml/mol	McGowan Method
pc	3872.29	kPa	Joback Method
ripol	1479.00		NIST Webbook
tb	431.24	K	Joback Method
tc	628.78	K	Joback Method
tf	222.51	K	Joback Method
vc	0.387	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	186.53	J/mol×K	431.24	Joback Method
cpg	195.71	J/mol×K	464.16	Joback Method
cpg	204.51	J/mol×K	497.09	Joback Method
cpg	212.94	J/mol×K	530.01	Joback Method
cpg	221.00	J/mol×K	562.93	Joback Method
cpg	228.69	J/mol×K	595.86	Joback Method
cpg	236.01	J/mol×K	628.78	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=R402190&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