2-[Pentylthio]ethanal

Inchi: InChI=1S/C7H14OS/c1-2-3-4-6-9-7-5-8/h5H,2-4,6-7H2,1H3
InchiKey: RVRKRAVIMVLTKL-UHFFFAOYSA-N
Formula: C7H14OS
SMILES: CCCCCSCC=O
Mol. weight [g/mol]: 146.25

Physical Properties

Property code	Value	Unit	Source
gf	-58.34	kJ/mol	Joback Method
hf	-231.52	kJ/mol	Joback Method
hfus	20.30	kJ/mol	Joback Method
hvap	44.71	kJ/mol	Joback Method
log10ws	-1.92		Crippen Method
logp	2.109		Crippen Method
mcvol	127.410	ml/mol	McGowan Method
pc	3089.85	kPa	Joback Method
ripol	1630.00		NIST Webbook
ripol	1630.00		NIST Webbook
tb	477.00	K	Joback Method
tc	670.16	K	Joback Method
tf	245.05	K	Joback Method
vc	0.498	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	265.83	J/mol×K	477.00	Joback Method
cpg	277.52	J/mol×K	509.19	Joback Method
cpg	288.70	J/mol×K	541.39	Joback Method
cpg	299.38	J/mol×K	573.58	Joback Method
cpg	309.57	J/mol×K	605.78	Joback Method
cpg	319.28	J/mol×K	637.97	Joback Method
cpg	328.52	J/mol×K	670.16	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=R402170&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