Acetic acid, thio-, S-hexyl ester

Inchi: InChI=1S/C8H16OS/c1-3-4-5-6-7-10-8(2)9/h3-7H2,1-2H3
InchiKey: UVOBMCVOACVTNV-UHFFFAOYSA-N
Formula: C8H16OS
SMILES: CCCCCCSC(C)=O
Mol. weight [g/mol]: 160.28
CAS: 2307-12-2

Physical Properties

Property code	Value	Unit	Source
gf	-79.32	kJ/mol	Joback Method
hf	-279.16	kJ/mol	Joback Method
hfus	22.20	kJ/mol	Joback Method
hvap	46.97	kJ/mol	Joback Method
log10ws	-2.83		Crippen Method
logp	2.846		Crippen Method
mcvol	141.500	ml/mol	McGowan Method
pc	2752.67	kPa	Joback Method
tb	505.09	K	Joback Method
tc	700.77	K	Joback Method
tf	264.25	K	Joback Method
vc	0.543	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	307.58	J/mol×K	505.09	Joback Method
cpg	320.67	J/mol×K	537.70	Joback Method
cpg	333.17	J/mol×K	570.32	Joback Method
cpg	345.09	J/mol×K	602.93	Joback Method
cpg	356.44	J/mol×K	635.54	Joback Method
cpg	367.24	J/mol×K	668.15	Joback Method
cpg	377.49	J/mol×K	700.77	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2307122&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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