2-[Prenylthio]ethanal

Inchi: InChI=1S/C7H12OS/c1-7(2)3-5-9-6-4-8/h3-4H,5-6H2,1-2H3
InchiKey: GZQSULYQPFAMJB-UHFFFAOYSA-N
Formula: C7H12OS
SMILES: CC(C)=CCSCC=O
Mol. weight [g/mol]: 144.24

Physical Properties

Property code	Value	Unit	Source
gf	13.33	kJ/mol	Joback Method
hf	-124.09	kJ/mol	Joback Method
hfus	19.20	kJ/mol	Joback Method
hvap	44.75	kJ/mol	Joback Method
log10ws	-1.77		Crippen Method
logp	1.885		Crippen Method
mcvol	123.110	ml/mol	McGowan Method
pc	3295.37	kPa	Joback Method
ripol	1673.00		NIST Webbook
ripol	1673.00		NIST Webbook
tb	481.04	K	Joback Method
tc	687.42	K	Joback Method
tf	226.01	K	Joback Method
vc	0.479	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	248.58	J/mol×K	481.04	Joback Method
cpg	259.98	J/mol×K	515.44	Joback Method
cpg	270.78	J/mol×K	549.83	Joback Method
cpg	281.00	J/mol×K	584.23	Joback Method
cpg	290.66	J/mol×K	618.63	Joback Method
cpg	299.78	J/mol×K	653.03	Joback Method
cpg	308.39	J/mol×K	687.42	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R402185&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

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