Propanethioic acid, S-propyl ester

Other names:	Propionic acid, thio-, S-propyl ester
	Propyl thiolpropionate
	Propyl thiopropionate
	S-propyl propanethioate
Inchi:	InChI=1S/C6H12OS/c1-3-5-8-6(7)4-2/h3-5H2,1-2H3
InchiKey:	CLBGDLKFLYZLDQ-UHFFFAOYSA-N
Formula:	C6H12OS
SMILES:	CCCSC(=O)CC
Mol. weight [g/mol]:	132.22
CAS:	2432-43-1

Physical Properties

Property code	Value	Unit	Source
gf	-96.16	kJ/mol	Joback Method
hf	-237.88	kJ/mol	Joback Method
hfus	17.03	kJ/mol	Joback Method
hvap	42.51	kJ/mol	Joback Method
log10ws	-1.99		Crippen Method
logp	2.066		Crippen Method
mcvol	113.320	ml/mol	McGowan Method
pc	3403.91	kPa	Joback Method
rinpol	943.00		NIST Webbook
tb	459.33	K	Joback Method
tc	660.04	K	Joback Method
tf	241.71	K	Joback Method
vc	0.431	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	223.40	J/mol×K	459.33	Joback Method
cpg	234.25	J/mol×K	492.78	Joback Method
cpg	244.63	J/mol×K	526.23	Joback Method
cpg	254.54	J/mol×K	559.69	Joback Method

cpg	264.00	J/mol×K	593.14	Joback Method
cpg	273.01	J/mol×K	626.59	Joback Method
cpg	281.57	J/mol×K	660.04	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2432431&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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