Propyl hydrodisulfide

Inchi: InChI=1S/C3H8S2/c1-2-3-5-4/h4H,2-3H2,1H3
InchiKey: HNXSKKGXEJGBFT-UHFFFAOYSA-N
Formula: C3H8S2
SMILES: CCCSS
Mol. weight [g/mol]: 108.23

Physical Properties

Property code	Value	Unit	Source
hf	-53.32	kJ/mol	Cheméo Relay (1.0)
hfus	11.70	kJ/mol	Joback Method
hvap	40.68	kJ/mol	Cheméo Relay (1.0)
ie	8.67	eV	Cheméo Relay (1.0)
log10ws	-2.03		Cheméo Relay (1.0)
logp	1.974		Crippen Method
mcvol	85.830	ml/mol	McGowan Method
rinpol	808.00		NIST Webbook
rinpol	865.20		NIST Webbook
rinpol	808.00		NIST Webbook
rinpol	865.20		NIST Webbook
tb	404.07	K	Cheméo Relay (1.0)
tc	652.33	K	Cheméo Relay (1.0)
tf	204.25	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	139.49	J/mol×K	399.68	Joback Method
cpg	147.23	J/mol×K	436.49	Joback Method
cpg	154.64	J/mol×K	473.30	Joback Method
cpg	161.74	J/mol×K	510.11	Joback Method
cpg	168.51	J/mol×K	546.92	Joback Method
cpg	174.97	J/mol×K	583.73	Joback Method
cpg	181.11	J/mol×K	620.54	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C137363849&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point