1,1-Propanedithiol

Inchi: InChI=1S/C3H8S2/c1-2-3(4)5/h3-5H,2H2,1H3
InchiKey: NCNISYUOWMIOPI-UHFFFAOYSA-N
Formula: C3H8S2
SMILES: CCC(S)S
Mol. weight [g/mol]: 108.23

Physical Properties

Property code	Value	Unit	Source
gf	30.72	kJ/mol	Joback Method
hf	-33.57	kJ/mol	Joback Method
hfus	8.09	kJ/mol	Joback Method
hvap	35.36	kJ/mol	Joback Method
log10ws	-1.83		Crippen Method
logp	1.582		Crippen Method
mcvol	85.830	ml/mol	McGowan Method
pc	5327.93	kPa	Joback Method
rinpol	839.00		NIST Webbook
rinpol	839.00		NIST Webbook
tb	393.32	K	Joback Method
tc	619.83	K	Joback Method
tf	181.49	K	Joback Method
vc	0.305	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	138.81	J/mol×K	393.32	Joback Method
cpg	146.84	J/mol×K	431.07	Joback Method
cpg	154.47	J/mol×K	468.82	Joback Method
cpg	161.70	J/mol×K	506.57	Joback Method
cpg	168.56	J/mol×K	544.33	Joback Method
cpg	175.04	J/mol×K	582.08	Joback Method
cpg	181.16	J/mol×K	619.83	Joback Method

Sources

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=R510840&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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