3-Thia-1-butanethiol

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

Physical Properties

Property code	Value	Unit	Source
gf	36.89	kJ/mol	Joback Method
hf	-24.90	kJ/mol	Joback Method
hfus	11.70	kJ/mol	Joback Method
hvap	35.83	kJ/mol	Joback Method
log10ws	-1.03		Crippen Method
logp	1.279		Crippen Method
mcvol	85.830	ml/mol	McGowan Method
pc	4924.59	kPa	Joback Method
rinpol	938.00		NIST Webbook
tb	399.68	K	Joback Method
tc	620.54	K	Joback Method
tf	194.43	K	Joback Method
vc	0.311	m3/kmol	Joback Method

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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R156793&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