3-Sulfanylbutan-1-ol

Inchi: InChI=1S/C4H10OS/c1-4(6)2-3-5/h4-6H,2-3H2,1H3
InchiKey: PHRRYVOQWOVNLF-UHFFFAOYSA-N
Formula: C4H10OS
SMILES: CC(S)CCO
Mol. weight [g/mol]: 106.19

Physical Properties

Property code	Value	Unit	Source
gf	-127.07	kJ/mol	Joback Method
hf	-244.92	kJ/mol	Joback Method
hfus	10.72	kJ/mol	Joback Method
hvap	47.53	kJ/mol	Joback Method
log10ws	-0.94		Crippen Method
logp	0.687		Crippen Method
mcvol	89.440	ml/mol	McGowan Method
pc	4835.95	kPa	Joback Method
rinpol	903.00		NIST Webbook
rinpol	903.00		NIST Webbook
ripol	1628.00		NIST Webbook
ripol	1628.00		NIST Webbook
tb	445.52	K	Joback Method
tc	633.53	K	Joback Method
tf	217.12	K	Joback Method
vc	0.327	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	173.64	J/mol×K	445.52	Joback Method
cpg	181.58	J/mol×K	476.85	Joback Method
cpg	189.18	J/mol×K	508.19	Joback Method
cpg	196.43	J/mol×K	539.52	Joback Method
cpg	203.36	J/mol×K	570.86	Joback Method
cpg	209.97	J/mol×K	602.19	Joback Method

cpg	216.27	J/mol×K	633.53	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=R621351&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume