3-Sulfanyl-2-butylpropanal

Inchi: InChI=1S/C7H14OS/c1-2-3-4-7(5-8)6-9/h5,7,9H,2-4,6H2,1H3
InchiKey: QEYQYTNODDKTJC-UHFFFAOYSA-N
Formula: C7H14OS
SMILES: CCCCC(C=O)CS
Mol. weight [g/mol]: 146.25

Physical Properties

Property code	Value	Unit	Source
gf	-64.51	kJ/mol	Joback Method
hf	-240.19	kJ/mol	Joback Method
hfus	16.69	kJ/mol	Joback Method
hvap	44.25	kJ/mol	Joback Method
log10ws	-1.86		Crippen Method
logp	1.921		Crippen Method
mcvol	127.410	ml/mol	McGowan Method
pc	3287.81	kPa	Joback Method
rinpol	1133.00		NIST Webbook
rinpol	1133.00		NIST Webbook
ripol	1659.00		NIST Webbook
tb	470.64	K	Joback Method
tc	668.23	K	Joback Method
tf	232.11	K	Joback Method
vc	0.492	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	264.16	J/mol×K	470.64	Joback Method
cpg	276.15	J/mol×K	503.57	Joback Method
cpg	287.57	J/mol×K	536.50	Joback Method
cpg	298.44	J/mol×K	569.43	Joback Method
cpg	308.78	J/mol×K	602.36	Joback Method
cpg	318.59	J/mol×K	635.29	Joback Method
cpg	327.90	J/mol×K	668.23	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R621242&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume