Rhodanine, 5-isopropylidene-

Inchi: InChI=1S/C6H7NOS2/c1-3(2)4-5(8)7-6(9)10-4/h1-2H3,(H,7,8,9)
InchiKey: MZEPNNPNBSNIER-UHFFFAOYSA-N
Formula: C6H7NOS2
SMILES: CC(C)=C1SC(=S)NC1=O
Mol. weight [g/mol]: 173.26
CAS: 28989-47-1

Physical Properties

Property code	Value	Unit	Source
gf	176.64	kJ/mol	Joback Method
hf	40.36	kJ/mol	Joback Method
hfus	21.96	kJ/mol	Joback Method
hvap	54.68	kJ/mol	Joback Method
log10ws	-2.77		Crippen Method
logp	1.428		Crippen Method
mcvol	120.190	ml/mol	McGowan Method
pc	4897.06	kPa	Joback Method
tb	599.99	K	Joback Method
tc	871.99	K	Joback Method
tf	489.29	K	Joback Method
vc	0.425	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	249.34	J/mol×K	599.99	Joback Method
cpg	259.70	J/mol×K	645.32	Joback Method
cpg	269.38	J/mol×K	690.66	Joback Method
cpg	278.41	J/mol×K	735.99	Joback Method
cpg	286.83	J/mol×K	781.32	Joback Method
cpg	294.66	J/mol×K	826.66	Joback Method
cpg	301.94	J/mol×K	871.99	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C28989471&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume