Rhodanine, 5-cinnamylidene-

Inchi: InChI=1S/C12H9NOS2/c14-11-10(16-12(15)13-11)8-4-7-9-5-2-1-3-6-9/h1-8H,(H,13,14,15
InchiKey: FPSVMWLWFSURME-WIXOJMCHSA-N
Formula: C12H9NOS2
SMILES: OC1=NC(=S)SC1=CC=Cc1ccccc1
Mol. weight [g/mol]: 247.34
CAS: 15328-87-7

Physical Properties

Property code	Value	Unit	Source
gf	463.51	kJ/mol	Joback Method
hf	345.00	kJ/mol	Joback Method
hfus	34.02	kJ/mol	Joback Method
hvap	83.03	kJ/mol	Joback Method
log10ws	-4.43		Crippen Method
logp	3.572		Crippen Method
mcvol	176.670	ml/mol	McGowan Method
pc	4041.50	kPa	Joback Method
tb	801.88	K	Joback Method
tc	1062.51	K	Joback Method
tf	564.60	K	Joback Method
vc	0.642	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	448.17	J/mol×K	801.88	Joback Method
cpg	458.30	J/mol×K	845.32	Joback Method
cpg	467.65	J/mol×K	888.76	Joback Method
cpg	476.38	J/mol×K	932.19	Joback Method
cpg	484.60	J/mol×K	975.63	Joback Method
cpg	492.45	J/mol×K	1019.07	Joback Method
cpg	500.06	J/mol×K	1062.51	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C15328877&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