Rhodanine, 5-(m-nitrobenzylidene)-

Inchi: InChI=1S/C10H6N2O3S2/c13-9-8(17-10(16)11-9)5-6-2-1-3-7(4-6)12(14)15/h1-5H,(H,11,
InchiKey: AVXJAQDWWJILLN-VMPITWQZSA-N
Formula: C10H6N2O3S2
SMILES: O=C1NC(=S)SC1=Cc1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]: 266.30
CAS: 6301-12-8

Physical Properties

Property code	Value	Unit	Source
gf	357.20	kJ/mol	Joback Method
hf	181.89	kJ/mol	Joback Method
hfus	38.65	kJ/mol	Joback Method
hvap	83.03	kJ/mol	Joback Method
log10ws	-4.37		Crippen Method
logp	2.084		Crippen Method
mcvol	170.210	ml/mol	McGowan Method
pc	4504.30	kPa	Joback Method
tb	875.13	K	Joback Method
tc	1185.79	K	Joback Method
tf	730.88	K	Joback Method
vc	0.623	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	429.68	J/mol×K	875.13	Joback Method
cpg	439.25	J/mol×K	926.91	Joback Method
cpg	447.78	J/mol×K	978.68	Joback Method
cpg	455.36	J/mol×K	1030.46	Joback Method
cpg	462.10	J/mol×K	1082.24	Joback Method
cpg	468.10	J/mol×K	1134.01	Joback Method
cpg	473.44	J/mol×K	1185.79	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=C6301128&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume