

5-Vanillylidene rhodanine

Inchi:	InChI=1S/C11H9NO3S2/c1-15-8-4-6(2-3-7(8)13)5-9-10(14)12-11(16)17-9/h2-5,13H,1H3
InchiKey:	OWXPWWRBBBGOLO-WEVVVXLNSA-N
Formula:	C11H9NO3S2
SMILES:	COc1cc(C=C2SC(=S)NC2=O)ccc1O
Mol. weight [g/mol]:	267.32
CAS:	5447-37-0

Physical Properties

Property code	Value	Unit	Source
gf	70.45	kJ/mol	Joback Method
hf	-137.52	kJ/mol	Joback Method
hfus	36.85	kJ/mol	Joback Method
hvap	84.09	kJ/mol	Joback Method
log10ws	-3.38		Crippen Method
logp	1.890		Crippen Method
mcvol	178.620	ml/mol	McGowan Method
pc	4652.99	kPa	Joback Method
tb	849.21	K	Joback Method
tc	1136.18	K	Joback Method
tf	732.49	K	Joback Method
vc	0.581	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	464.18	J/molxK	849.21	Joback Method
cpg	475.30	J/molxK	897.04	Joback Method
cpg	485.80	J/molxK	944.87	Joback Method
cpg	495.80	J/molxK	992.69	Joback Method
cpg	505.42	J/molxK	1040.52	Joback Method
cpg	514.79	J/molxK	1088.35	Joback Method
cpg	524.02	J/molxK	1136.18	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=C5447370&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

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