5-(4-Diethylaminobenzylidene)rhodanine

Other names:	p-Diethylaminobenzylidene rhodanine
	4-Thiazolidinone, 5-[[4-(diethylamino)phenyl]methylene]-2-thioxo-
	5-(p-(Diethylamino)benzylidene)rhodanine
	5-[p-(diethylamino)benzylidene]-2-thioxothiazolidin-4-one
Inchi:	InChI=1S/C14H16N2OS2/c1-3-16(4-2)11-7-5-10(6-8-11)9-12-13(17)15-14(18)19-12/h5-9
InchiKey:	CWQLQYNQWCTDQF-FMIVXFBMSA-N
Formula:	C14H16N2OS2
SMILES:	CCN(CC)c1ccc(C=C2SC(=S)NC2=O)cc1
Mol. weight [g/mol]:	292.42
CAS:	35778-58-6

Physical Properties

Property code	Value	Unit	Source
gf	466.11	kJ/mol	Joback Method
hf	177.62	kJ/mol	Joback Method
hfus	40.67	kJ/mol	Joback Method
hvap	77.39	kJ/mol	Joback Method
log10ws	-4.46		Crippen Method
logp	3.022		Crippen Method
mcvol	219.130	ml/mol	McGowan Method
pc	2805.41	kPa	Joback Method
tb	827.25	K	Joback Method
tc	1090.66	K	Joback Method
tf	664.82	K	Joback Method
vc	0.782	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	599.29	J/mol×K	827.25	Joback Method
cpg	613.55	J/mol×K	871.15	Joback Method
cpg	626.67	J/mol×K	915.05	Joback Method
cpg	638.75	J/mol×K	958.96	Joback Method
cpg	649.87	J/mol×K	1002.86	Joback Method

cpg	660.13	J/mol×K	1046.76	Joback Method
cpg	669.63	J/mol×K	1090.66	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C35778586&Units=SI

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