

p-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=C2/SC(=S)NC2=O)cc1
Mol. weight [g/mol]:	292.43

Physical Properties

Property code	Value	Unit	Source
hfus	40.67	kJ/mol	Joback Method
logp	3.022		Crippen Method
mcvol	219.130	ml/mol	McGowan Method
tf	474.75	K	Cheméo Relay (1.0)

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

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

Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

cpg: Ideal gas heat capacity
hfus: Enthalpy of fusion at standard conditions
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tf: Normal melting (fusion) point

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