2,8-Dioctyl phenothiazine

Inchi: InChI=1S/C28H41NS/c1-3-5-7-9-11-13-15-23-17-19-27-25(21-23)29-26-22-24(18-20-28(
InchiKey: QYZRFLASALOUKY-UHFFFAOYSA-N
Formula: C28H41NS
SMILES: CCCCCCCCc1ccc2c(c1)Nc1cc(CCCCCCCC)ccc1S2
Mol. weight [g/mol]: 423.70
CAS: 84460-70-8

Physical Properties

Property code	Value	Unit	Source
gf	579.31	kJ/mol	Joback Method
hf	-11.70	kJ/mol	Joback Method
hfus	67.21	kJ/mol	Joback Method
hvap	97.74	kJ/mol	Joback Method
log10ws	-10.57		Crippen Method
logp	9.701		Crippen Method
mcvol	373.330	ml/mol	McGowan Method
pc	1009.73	kPa	Joback Method
tb	1016.84	K	Joback Method
tc	1247.32	K	Joback Method
tf	722.42	K	Joback Method
vc	1.437	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1252.32	J/mol×K	1016.84	Joback Method
cpg	1271.71	J/mol×K	1055.25	Joback Method
cpg	1290.26	J/mol×K	1093.67	Joback Method
cpg	1308.11	J/mol×K	1132.08	Joback Method
cpg	1325.38	J/mol×K	1170.49	Joback Method
cpg	1342.23	J/mol×K	1208.90	Joback Method
cpg	1358.78	J/mol×K	1247.32	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=C84460708&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

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