Disulfide, bis(p-chloro acetamido phenyl)

Inchi: InChI=1S/C16H14Cl2N2O2S2/c17-9-15(21)19-11-1-5-13(6-2-11)23-24-14-7-3-12(4-8-14
InchiKey: KSQWUMVUPBMLKB-UHFFFAOYSA-N
Formula: C16H14Cl2N2O2S2
SMILES: O=C(CCl)Nc1ccc(SSc2ccc(NC(=O)CCl)cc2)cc1
Mol. weight [g/mol]: 401.33
CAS: 6339-52-2

Physical Properties

Property code	Value	Unit	Source
gf	252.72	kJ/mol	Joback Method
hf	10.59	kJ/mol	Joback Method
hfus	54.55	kJ/mol	Joback Method
hvap	105.85	kJ/mol	Joback Method
log10ws	-5.47		Crippen Method
logp	4.841		Crippen Method
mcvol	269.060	ml/mol	McGowan Method
pc	2475.19	kPa	Joback Method
tb	1049.30	K	Joback Method
tc	1317.20	K	Joback Method
tf	681.78	K	Joback Method
vc	1.004	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	731.90	J/mol×K	1049.30	Joback Method
cpg	738.38	J/mol×K	1093.95	Joback Method
cpg	743.60	J/mol×K	1138.60	Joback Method
cpg	747.64	J/mol×K	1183.25	Joback Method
cpg	750.58	J/mol×K	1227.90	Joback Method
cpg	752.50	J/mol×K	1272.55	Joback Method
cpg	753.46	J/mol×K	1317.20	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6339522&Units=SI
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

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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