l-Cysteine, N,S-bis(m-toluoyl)-, methyl ester

Inchi: InChI=1S/C20H21NO4S/c1-13-6-4-8-15(10-13)18(22)21-17(19(23)25-3)12-26-20(24)16-9
InchiKey: ZNBCBVIRCCFBAN-UHFFFAOYSA-N
Formula: C20H21NO4S
SMILES: COC(=O)C(CSC(=O)c1cccc(C)c1)NC(=O)c1cccc(C)c1
Mol. weight [g/mol]: 371.45

Physical Properties

Property code	Value	Unit	Source
gf	-48.61	kJ/mol	Joback Method
hf	-385.91	kJ/mol	Joback Method
hfus	46.55	kJ/mol	Joback Method
hvap	101.50	kJ/mol	Joback Method
log10ws	-5.27		Crippen Method
logp	3.148		Crippen Method
mcvol	282.050	ml/mol	McGowan Method
pc	1896.95	kPa	Joback Method
rinpol	2973.00		NIST Webbook
tb	1022.86	K	Joback Method
tc	1271.06	K	Joback Method
tf	637.12	K	Joback Method
vc	1.058	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	863.48	J/mol×K	1022.86	Joback Method
cpg	872.96	J/mol×K	1064.23	Joback Method
cpg	880.98	J/mol×K	1105.59	Joback Method
cpg	887.59	J/mol×K	1146.96	Joback Method
cpg	892.86	J/mol×K	1188.33	Joback Method
cpg	896.82	J/mol×K	1229.70	Joback Method
cpg	899.55	J/mol×K	1271.06	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=U299643&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume