N-1-[1,1-bis(acetylmercaptomethyl)propyl]-p-tolue

Inchi: InChI=1S/C16H23NO4S3/c1-5-16(10-22-13(3)18,11-23-14(4)19)17-24(20,21)15-8-6-12(2
InchiKey: WLJSXBZFXPVMAO-UHFFFAOYSA-N
Formula: C16H23NO4S3
SMILES: CCC(CSC(C)=O)(CSC(C)=O)NS(=O)(=O)c1ccc(C)cc1
Mol. weight [g/mol]: 389.55
CAS: 10405-53-5

Physical Properties

Property code	Value	Unit	Source
gf	-381.29	kJ/mol	Joback Method
hf	-698.56	kJ/mol	Joback Method
hfus	51.37	kJ/mol	Joback Method
hvap	105.05	kJ/mol	Joback Method
log10ws	-4.60		Crippen Method
logp	2.982		Crippen Method
mcvol	286.450	ml/mol	McGowan Method
pc	2287.14	kPa	Joback Method
tb	937.16	K	Joback Method
tc	1172.16	K	Joback Method
tf	571.32	K	Joback Method
vc	1.093	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	845.34	J/mol×K	937.16	Joback Method
cpg	856.18	J/mol×K	976.33	Joback Method
cpg	865.56	J/mol×K	1015.49	Joback Method
cpg	873.51	J/mol×K	1054.66	Joback Method
cpg	880.08	J/mol×K	1093.83	Joback Method
cpg	885.31	J/mol×K	1133.00	Joback Method
cpg	889.26	J/mol×K	1172.16	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10405535&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