2-Methyl-2-p-toluenesulfonylamino-1,3-propanedi diacetate

InChI: InChI=1S/C15H21NO4S3/c1-11-5-7-14(8-6-11)23(19,20)16-15(4,9-21-12(2)17)10-22-13(

InChIKey: UTPPLRNAHYCAGV-UHFFFAOYSA-N

Formula: C15H21NO4S3

SMILES: CC(=O)SCC(C)(CSC(C)=O)NS(=O)(=O)c1ccc(C)cc1

Mol. weight [g/mol]: 375.53

CAS: 10405-54-6

Physical Properties

Property code	Value	Unit	Source
gf	-389.71	kJ/mol	Joback Method
hf	-677.92	kJ/mol	Joback Method
hfus	48.78	kJ/mol	Joback Method
hvap	102.82	kJ/mol	Joback Method
log10ws	-4.18		Crippen Method
logp	2.591		Crippen Method
mcvol	272.360	ml/mol	McGowan Method
pc	2512.55	kPa	Joback Method
tb	914.28	K	Joback Method
tc	1151.22	K	Joback Method
tf	560.05	K	Joback Method
vc	1.038	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	788.73	J/mol×K	914.28	Joback Method
cpg	799.58	J/mol×K	953.77	Joback Method
cpg	808.97	J/mol×K	993.26	Joback Method
cpg	816.95	J/mol×K	1032.75	Joback Method
cpg	823.55	J/mol×K	1072.24	Joback Method
cpg	828.81	J/mol×K	1111.73	Joback Method
cpg	832.79	J/mol×K	1151.22	Joback Method

Sources

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=C10405546&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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