1-Amino-2-methoxy-4-p-tolylsulfonamido-anthraq

Other names: N-(4-amino-9,10-dihydro-3-methoxy-9,10-dioxo-1-anthryl)-4-methylbenzenesulphonamide
Inchi: InChI=1S/C22H18N2O5S/c1-12-7-9-13(10-8-12)30(27,28)24-16-11-17(29-2)20(23)19-18
InchiKey: BXIGAWRFDMDLTL-UHFFFAOYSA-N
Formula: C22H18N2O5S
SMILES: COc1cc(NS(=O)(=O)c2ccc(C)cc2)c2c(c1N)C(=O)c1ccccc1C2=O
Mol. weight [g/mol]: 422.45
CAS: 81-68-5

Physical Properties

Property code	Value	Unit	Source
gf	-168.51	kJ/mol	Joback Method
hf	-531.05	kJ/mol	Joback Method
hfus	53.57	kJ/mol	Joback Method
hvap	122.03	kJ/mol	Joback Method
log10ws	-5.37		Crippen Method
logp	3.162		Crippen Method
mcvol	295.760	ml/mol	McGowan Method
pc	2472.73	kPa	Joback Method
tb	1148.36	K	Joback Method
tc	1418.14	K	Joback Method
tf	850.93	K	Joback Method
vc	1.131	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	937.98	J/mol×K	1148.36	Joback Method
cpg	941.29	J/mol×K	1193.32	Joback Method
cpg	942.30	J/mol×K	1238.29	Joback Method
cpg	941.02	J/mol×K	1283.25	Joback Method
cpg	937.45	J/mol×K	1328.21	Joback Method
cpg	931.61	J/mol×K	1373.17	Joback Method
cpg	923.49	J/mol×K	1418.14	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=C81685&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume