N-m-Tolyloxyacetyl-benzenesulfonamide

Inchi: InChI=1S/C15H15NO4S/c1-12-6-5-7-13(10-12)20-11-15(17)16-21(18,19)14-8-3-2-4-9-14
InchiKey: SFZYHNAGMAZZMB-UHFFFAOYSA-N
Formula: C15H15NO4S
SMILES: Cc1cccc(OCC(=O)NS(=O)(=O)c2ccccc2)c1
Mol. weight [g/mol]: 305.35
CAS: 17811-69-7

Physical Properties

Property code	Value	Unit	Source
gf	-322.46	kJ/mol	Joback Method
hf	-536.02	kJ/mol	Joback Method
hfus	41.56	kJ/mol	Joback Method
hvap	88.42	kJ/mol	Joback Method
log10ws	-3.36		Crippen Method
logp	1.879		Crippen Method
mcvol	220.200	ml/mol	McGowan Method
pc	3096.73	kPa	Joback Method
rinpol	2528.00		NIST Webbook
rinpol	2528.00		NIST Webbook
tb	775.18	K	Joback Method
tc	1002.12	K	Joback Method
tf	487.55	K	Joback Method
vc	0.845	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	604.89	J/mol×K	775.18	Joback Method
cpg	618.42	J/mol×K	813.00	Joback Method
cpg	630.66	J/mol×K	850.83	Joback Method
cpg	641.62	J/mol×K	888.65	Joback Method
cpg	651.33	J/mol×K	926.47	Joback Method
cpg	659.82	J/mol×K	964.29	Joback Method
cpg	667.12	J/mol×K	1002.12	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17811697&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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