

N-m-Tolyloxyacetyl-benzenesulfonamide, N-methyl-

Inchi: InChI=1S/C16H17NO4S/c1-13-7-6-8-14(11-13)21-12-16(18)17(2)22(19,20)15-9-4-3-5-10

InchiKey: NIFVWHDESDPHMN-UHFFFAOYSA-N

Formula: C16H17NO4S

SMILES: Cc1cccc(OCC(=O)N(C)S(=O)(=O)c2ccccc2)c1

Mol. weight [g/mol]: 319.38

Physical Properties

Property code	Value	Unit	Source
gf	-292.65	kJ/mol	Joback Method
hf	-542.60	kJ/mol	Joback Method
hfus	42.07	kJ/mol	Joback Method
hvap	86.26	kJ/mol	Joback Method
log10ws	-3.16		Crippen Method
logp	2.221		Crippen Method
mcvol	234.290	ml/mol	McGowan Method
pc	2746.90	kPa	Joback Method
rinpol	2537.00		NIST Webbook
rinpol	2537.00		NIST Webbook
tb	760.33	K	Joback Method
tc	982.13	K	Joback Method
tf	478.63	K	Joback Method
vc	0.883	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	645.95	J/mol×K	760.33	Joback Method
cpg	660.77	J/mol×K	797.30	Joback Method
cpg	674.26	J/mol×K	834.26	Joback Method
cpg	686.47	J/mol×K	871.23	Joback Method
cpg	697.43	J/mol×K	908.20	Joback Method
cpg	707.17	J/mol×K	945.16	Joback Method
cpg	715.74	J/mol×K	982.13	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374385&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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