2-Methylbenzene-1,4-diamine, N1,N3,N3-triacetyl-

Inchi: InChI=1S/C13H16N2O3/c1-8-7-12(15(10(3)17)11(4)18)5-6-13(8)14-9(2)16/h5-7H,1-4H3,

InchiKey: ZRALWTXFYYXZEN-UHFFFAOYSA-N

Formula: C13H16N2O3

SMILES: CC(=O)Nc1ccc(N(C(C)=O)C(C)=O)cc1C

Mol. weight [g/mol]: 248.28

Physical Properties

Property code	Value	Unit	Source
gf	-34.86	kJ/mol	Joback Method
hf	-314.80	kJ/mol	Joback Method
hfus	35.61	kJ/mol	Joback Method
hvap	76.85	kJ/mol	Joback Method
log10ws	-2.45		Crippen Method
logp	1.853		Crippen Method
mcvol	194.940	ml/mol	McGowan Method
pc	2589.85	kPa	Joback Method
rinpol	2184.00		NIST Webbook
rinpol	2184.00		NIST Webbook
tb	757.70	K	Joback Method
tc	974.50	K	Joback Method
tf	522.65	K	Joback Method
vc	0.727	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	539.93	J/mol×K	757.70	Joback Method
cpg	552.44	J/mol×K	793.83	Joback Method
cpg	564.02	J/mol×K	829.97	Joback Method
cpg	574.73	J/mol×K	866.10	Joback Method
cpg	584.59	J/mol×K	902.24	Joback Method
cpg	593.66	J/mol×K	938.37	Joback Method
cpg	601.96	J/mol×K	974.50	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=U373215&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume