

4-Methoxybenzene-1,3-diamine, N1,N1,N3,N3-tetraacetyl-

Inchi: InChI=1S/C15H18N2O5/c1-9(18)16(10(2)19)13-6-7-15(22-5)14(8-13)17(11(3)20)12(4)21
InchiKey: KRBQLADALVNGTP-UHFFFAOYSA-N
Formula: C15H18N2O5
SMILES: COc1ccc(N(C(C)=O)C(C)=O)cc1N(C(C)=O)C(C)=O
Mol. weight [g/mol]: 306.31

Physical Properties

Property code	Value	Unit	Source
gf	-230.55	kJ/mol	Joback Method
hf	-586.82	kJ/mol	Joback Method
hfus	41.49	kJ/mol	Joback Method
hvap	86.06	kJ/mol	Joback Method
log10ws	-2.18		Crippen Method
logp	1.494		Crippen Method
mcvol	230.560	ml/mol	McGowan Method
pc	2212.45	kPa	Joback Method
rinpol	2155.00		NIST Webbook
tb	842.02	K	Joback Method
tc	1056.92	K	Joback Method
tf	597.16	K	Joback Method
vc	0.846	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	674.22	J/mol×K	842.02	Joback Method
cpg	686.10	J/mol×K	877.84	Joback Method
cpg	696.97	J/mol×K	913.65	Joback Method
cpg	706.86	J/mol×K	949.47	Joback Method
cpg	715.81	J/mol×K	985.29	Joback Method
cpg	723.85	J/mol×K	1021.11	Joback Method
cpg	731.02	J/mol×K	1056.92	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373465&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

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