

4-[1-Acetoxy-2-(diacetylamino)ethyl]phenyl acetate

Other names:	1-(4-Acetyloxyphenyl)-2-diacetylaminoethanol acetate 4-[2-Diacetylamino-1-acetyloxyethyl]phenol acetate
Inchi:	InChI=1S/C16H19NO6/c1-10(18)17(11(2)19)9-16(23-13(4)21)14-5-7-15(8-6-14)22-12(3)
InchiKey:	WXBPPNDYHGULCD-UHFFFAOYSA-N
Formula:	C16H19NO6
SMILES:	CC(=O)Oc1ccc(C(CN(C(C)=O)C(C)=O)OC(C)=O)cc1
Mol. weight [g/mol]:	321.33

Physical Properties

Property code	Value	Unit	Source
gf	-430.72	kJ/mol	Joback Method
hf	-801.02	kJ/mol	Joback Method
hfus	39.12	kJ/mol	Joback Method
hvap	87.61	kJ/mol	Joback Method
log10ws	-2.54		Crippen Method
logp	1.611		Crippen Method
mcvol	240.540	ml/mol	McGowan Method
pc	2040.07	kPa	Joback Method
rinpol	2304.00		NIST Webbook
tb	869.46	K	Joback Method
tc	1085.87	K	Joback Method
tf	570.67	K	Joback Method
vc	0.895	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	717.55	J/molxK	869.46	Joback Method
cpg	729.33	J/molxK	905.53	Joback Method
cpg	739.98	J/molxK	941.60	Joback Method
cpg	749.51	J/molxK	977.67	Joback Method
cpg	757.94	J/molxK	1013.73	Joback Method
cpg	765.30	J/molxK	1049.80	Joback Method
cpg	771.60	J/molxK	1085.87	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373313&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
hvp:	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
rlnol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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