2,4-Diaminophenol, N,N',O-triacetyl-

Other names: 2,4-Diacetamidophenyl acetate
Inchi: InChI=1S/C12H14N2O4/c1-7(15)13-10-4-5-12(18-9(3)17)11(6-10)14-8(2)16/h4-6H,1-3H
InchiKey: CFSQVTPCXOCSIL-UHFFFAOYSA-N
Formula: C12H14N2O4
SMILES: CC(=O)Nc1ccc(OC(C)=O)c(NC(C)=O)c1
Mol. weight [g/mol]: 250.25

Physical Properties

Property code	Value	Unit	Source
gf	-169.67	kJ/mol	Joback Method
hf	-440.44	kJ/mol	Joback Method
hfus	36.28	kJ/mol	Joback Method
hvap	81.43	kJ/mol	Joback Method
log10ws	-2.19		Crippen Method
logp	1.529		Crippen Method
mcvol	186.720	ml/mol	McGowan Method
pc	2856.62	kPa	Joback Method
rinpol	2341.00		NIST Webbook
tb	794.97	K	Joback Method
tc	1014.83	K	Joback Method
tf	553.80	K	Joback Method
vc	0.706	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	522.95	J/mol×K	794.97	Joback Method
cpg	533.99	J/mol×K	831.61	Joback Method
cpg	544.11	J/mol×K	868.26	Joback Method
cpg	553.33	J/mol×K	904.90	Joback Method
cpg	561.66	J/mol×K	941.54	Joback Method
cpg	569.12	J/mol×K	978.19	Joback Method
cpg	575.72	J/mol×K	1014.83	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373245&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