Pentanedioic acid, 2-benzoylamino, dimethyl ester

Inchi: InChI=1S/C14H17NO5/c1-19-12(16)9-8-11(14(18)20-2)15-13(17)10-6-4-3-5-7-10/h3-7,11

InchiKey: JOTSRQZZNLVBKG-UHFFFAOYSA-N

Formula: C14H17NO5

SMILES: COC(=O)CCC(NC(=O)c1ccccc1)C(=O)OC

Mol. weight [g/mol]: 279.29

Physical Properties

Property code	Value	Unit	Source
gf	-330.40	kJ/mol	Joback Method
hf	-649.75	kJ/mol	Joback Method
hfus	34.81	kJ/mol	Joback Method
hvap	80.14	kJ/mol	Joback Method
log10ws	-2.16		Crippen Method
logp	0.911		Crippen Method
mcvol	210.790	ml/mol	McGowan Method
pc	2367.97	kPa	Joback Method
rinpol	2110.00		NIST Webbook
rinpol	2110.00		NIST Webbook
tb	802.58	K	Joback Method
tc	1017.62	K	Joback Method
tf	505.87	K	Joback Method
vc	0.794	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	609.10	J/mol×K	802.58	Joback Method
cpg	621.48	J/mol×K	838.42	Joback Method
cpg	632.82	J/mol×K	874.26	Joback Method
cpg	643.13	J/mol×K	910.10	Joback Method
cpg	652.43	J/mol×K	945.94	Joback Method
cpg	660.72	J/mol×K	981.78	Joback Method
cpg	668.03	J/mol×K	1017.62	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=R106659&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