[4-[2-(Methoxycarbonylamino)ethyl]phenyl] methyl carbonate

Inchi: InChI=1S/C12H15NO5/c1-16-11(14)13-8-7-9-3-5-10(6-4-9)18-12(15)17-2/h3-6H,7-8H2,1

InchiKey: XXRVWYOAMHOXJI-UHFFFAOYSA-N

Formula: C12H15NO5

SMILES: COC(=O)NCCc1ccc(OC(=O)OC)cc1

Mol. weight [g/mol]: 253.25

Physical Properties

Property code	Value	Unit	Source
gf	-330.51	kJ/mol	Joback Method
hf	-634.30	kJ/mol	Joback Method
hfus	32.35	kJ/mol	Joback Method
hvap	72.40	kJ/mol	Joback Method
log10ws	-2.52		Crippen Method
logp	1.730		Crippen Method
mcvol	186.910	ml/mol	McGowan Method
pc	2587.22	kPa	Joback Method
rinpol	2015.00		NIST Webbook
tb	730.79	K	Joback Method
tc	940.38	K	Joback Method
tf	483.15	K	Joback Method
vc	0.701	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	512.91	J/mol×K	730.79	Joback Method
cpg	525.59	J/mol×K	765.72	Joback Method
cpg	537.39	J/mol×K	800.65	Joback Method
cpg	548.29	J/mol×K	835.58	Joback Method
cpg	558.29	J/mol×K	870.51	Joback Method
cpg	567.37	J/mol×K	905.44	Joback Method
cpg	575.53	J/mol×K	940.38	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R577878&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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