3-phenylprop-2-enyl 2-aminobenzoate

Inchi: InChI=1S/C16H15NO2/c17-15-11-5-4-10-14(15)16(18)19-12-6-9-13-7-2-1-3-8-13/h1-11H
InchiKey: GABQNAFEZZDSCM-UHFFFAOYSA-N
Formula: C16H15NO2
SMILES: Nc1ccccc1C(=O)OCC=Cc1ccccc1
Mol. weight [g/mol]: 253.30

Physical Properties

Property code	Value	Unit	Source
gf	211.78	kJ/mol	Joback Method
hf	-5.77	kJ/mol	Joback Method
hfus	33.07	kJ/mol	Joback Method
hvap	76.18	kJ/mol	Joback Method
log10ws	-6.04		Aqueous Solubility Prediction Method
logp	3.139		Crippen Method
mcvol	201.900	ml/mol	McGowan Method
pc	2624.46	kPa	Joback Method
tb	776.80	K	Joback Method
tc	1024.47	K	Joback Method
tf	485.78	K	Joback Method
vc	0.749	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	554.80	J/mol×K	776.80	Joback Method
cpg	568.83	J/mol×K	818.08	Joback Method
cpg	581.66	J/mol×K	859.36	Joback Method
cpg	593.39	J/mol×K	900.64	Joback Method
cpg	604.10	J/mol×K	941.92	Joback Method
cpg	613.87	J/mol×K	983.20	Joback Method
cpg	622.79	J/mol×K	1024.47	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume