Heptyl p-aminobenzoate

Other names: heptyl-4-aminobenzoate
Inchi: InChI=1S/C14H21NO2/c1-2-3-4-5-6-11-17-14(16)12-7-9-13(15)10-8-12/h7-10H,2-6,11,15
InchiKey: IAHJVNSZPMIREM-UHFFFAOYSA-N
Formula: C14H21NO2
SMILES: CCCCCCCOC(=O)c1ccc(N)cc1
Mol. weight [g/mol]: 235.32

Physical Properties

Property code	Value	Unit	Source
gf	2.31	kJ/mol	Joback Method
hf	-318.24	kJ/mol	Joback Method
hfus	33.65	kJ/mol	Joback Method
hvap	69.49	kJ/mol	Joback Method
log10ws	-4.60		Aqueous Solubility Prediction Method
logp	3.396		Crippen Method
mcvol	201.780	ml/mol	McGowan Method
pc	2177.49	kPa	Joback Method
rinpol	2046.00		NIST Webbook
rinpol	2046.00		NIST Webbook
rinpol	2054.00		NIST Webbook
tb	700.20	K	Joback Method
tc	908.41	K	Joback Method
tf	441.90	K	Joback Method
vc	0.764	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	559.99	J/mol×K	700.20	Joback Method
cpg	575.33	J/mol×K	734.90	Joback Method
cpg	589.73	J/mol×K	769.60	Joback Method
cpg	603.22	J/mol×K	804.31	Joback Method
cpg	615.83	J/mol×K	839.01	Joback Method

cpg	627.58	J/mol×K	873.71	Joback Method
cpg	638.51	J/mol×K	908.41	Joback Method

Sources

Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R578831&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
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