benzoic acid, 4-amino-, hexyl ester

Other names: hexyl 4-aminobenzoate
Hexyl p-aminobenzoate
Inchi: InChI=1S/C13H19NO2/c1-2-3-4-5-10-16-13(15)11-6-8-12(14)9-7-11/h6-9H,2-5,10,14H2,
InchiKey: UWIGKXXCHKVGHW-UHFFFAOYSA-N
Formula: C13H19NO2
SMILES: CCCCCCOC(=O)c1ccc(N)cc1
Mol. weight [g/mol]: 221.30

Physical Properties

Property code	Value	Unit	Source
gf	-6.11	kJ/mol	Joback Method
hf	-297.60	kJ/mol	Joback Method
hfus	31.06	kJ/mol	Joback Method
hvap	67.27	kJ/mol	Joback Method
log10ws	-3.44		Crippen Method
logp	3.006		Crippen Method
mcvol	187.690	ml/mol	McGowan Method
pc	2386.52	kPa	Joback Method
rinpol	1956.00		NIST Webbook
rinpol	1956.00		NIST Webbook
rinpol	1955.00		NIST Webbook
tb	677.32	K	Joback Method
tc	888.49	K	Joback Method
tf	430.63	K	Joback Method
vc	0.709	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	507.18	J/mol×K	677.32	Joback Method
cpg	522.08	J/mol×K	712.51	Joback Method
cpg	536.07	J/mol×K	747.71	Joback Method
cpg	549.17	J/mol×K	782.90	Joback Method
cpg	561.42	J/mol×K	818.10	Joback Method

cpg	572.83	J/mol×K	853.29	Joback Method
cpg	583.43	J/mol×K	888.49	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=U400807&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