Benzoic acid, 4-amino-, octyl ester

Other names: octyl-4-aminobenzoate
Inchi: InChI=1S/C15H23NO2/c1-2-3-4-5-6-7-12-18-15(17)13-8-10-14(16)11-9-13/h8-11H,2-7,1
InchiKey: XOEUGELJHSUYGP-UHFFFAOYSA-N
Formula: C15H23NO2
SMILES: CCCCCCCCOC(=O)c1ccc(N)cc1
Mol. weight [g/mol]: 249.35
CAS: 14309-41-2

Physical Properties

Property code	Value	Unit	Source
gf	10.73	kJ/mol	Joback Method
hf	-338.88	kJ/mol	Joback Method
hfus	36.24	kJ/mol	Joback Method
hvap	71.72	kJ/mol	Joback Method
log10ws	-5.40		Aqueous Solubility Prediction Method
logp	3.786		Crippen Method
mcvol	215.870	ml/mol	McGowan Method
pc	1994.77	kPa	Joback Method
rinpol	2144.00		NIST Webbook
rinpol	2153.00		NIST Webbook
rinpol	2144.00		NIST Webbook
tb	723.08	K	Joback Method
tc	928.76	K	Joback Method
tf	345.00 ± 1.00	K	NIST Webbook
vc	0.821	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	614.05	J/mol×K	723.08	Joback Method
cpg	629.76	J/mol×K	757.36	Joback Method
cpg	644.51	J/mol×K	791.64	Joback Method
cpg	658.33	J/mol×K	825.92	Joback Method

cpg	671.24	J/mol×K	860.20	Joback Method
cpg	683.28	J/mol×K	894.48	Joback Method
cpg	694.46	J/mol×K	928.76	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C14309412&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