Benzoic acid, 3-(propylamino)-, methyl ester

Inchi: InChI=1S/C11H15NO2/c1-3-7-12-10-6-4-5-9(8-10)11(13)14-2/h4-6,8,12H,3,7H2,1-2H3
InchiKey: GYNRHKAFZOFCID-UHFFFAOYSA-N
Formula: C11H15NO2
SMILES: CCCNc1cccc(C(=O)OC)c1
Mol. weight [g/mol]: 193.24

Physical Properties

Property code	Value	Unit	Source
gf	-0.01	kJ/mol	Joback Method
hf	-236.64	kJ/mol	Joback Method
hfus	25.78	kJ/mol	Joback Method
hvap	58.61	kJ/mol	Joback Method
log10ws	-2.56		Crippen Method
logp	2.295		Crippen Method
mcvol	159.510	ml/mol	McGowan Method
pc	2773.00	kPa	Joback Method
rinpol	1698.00		NIST Webbook
rinpol	1698.00		NIST Webbook
tb	609.20	K	Joback Method
tc	819.40	K	Joback Method
tf	377.49	K	Joback Method
vc	0.603	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	395.72	J/mol×K	609.20	Joback Method
cpg	409.76	J/mol×K	644.23	Joback Method
cpg	422.99	J/mol×K	679.27	Joback Method
cpg	435.44	J/mol×K	714.30	Joback Method
cpg	447.11	J/mol×K	749.33	Joback Method
cpg	458.03	J/mol×K	784.36	Joback Method
cpg	468.21	J/mol×K	819.40	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374486&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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