Methyl 2-(isopentylamino)benzoate

Inchi: InChI=1S/C13H19NO2/c1-10(2)8-9-14-12-7-5-4-6-11(12)13(15)16-3/h4-7,10,14H,8-9H2,
InchiKey: IIWKDYNSYHLHNY-UHFFFAOYSA-N
Formula: C13H19NO2
SMILES: COC(=O)c1ccccc1NCCC(C)C
Mol. weight [g/mol]: 221.30
CAS: 893729-04-9

Physical Properties

Property code	Value	Unit	Source
gf	14.39	kJ/mol	Joback Method
hf	-283.20	kJ/mol	Joback Method
hfus	27.44	kJ/mol	Joback Method
hvap	62.67	kJ/mol	Joback Method
log10ws	-3.16		Crippen Method
logp	2.931		Crippen Method
mcvol	187.690	ml/mol	McGowan Method
pc	2304.74	kPa	Joback Method
rinpol	1854.50		NIST Webbook
rinpol	1854.50		NIST Webbook
tb	654.52	K	Joback Method
tc	862.27	K	Joback Method
tf	385.03	K	Joback Method
vc	0.709	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	497.02	J/mol×K	654.52	Joback Method
cpg	512.54	J/mol×K	689.15	Joback Method
cpg	527.14	J/mol×K	723.77	Joback Method
cpg	540.84	J/mol×K	758.40	Joback Method
cpg	553.67	J/mol×K	793.02	Joback Method
cpg	565.65	J/mol×K	827.65	Joback Method
cpg	576.80	J/mol×K	862.27	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C893729049&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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume