Butyl 3-iodobenzoate

Inchi: InChI=1S/C11H13IO2/c1-2-3-7-14-11(13)9-5-4-6-10(12)8-9/h4-6,8H,2-3,7H2,1H3
InchiKey: WVGMCYXQJIQRAR-UHFFFAOYSA-N
Formula: C11H13IO2
SMILES: CCCCOC(=O)c1cccc(I)c1
Mol. weight [g/mol]: 304.12

Physical Properties

Property code	Value	Unit	Source
gf	-31.28	kJ/mol	Joback Method
hf	-213.24	kJ/mol	Joback Method
hfus	25.09	kJ/mol	Joback Method
hvap	61.55	kJ/mol	Joback Method
log10ws	-4.12		Crippen Method
logp	3.248		Crippen Method
mcvol	175.350	ml/mol	McGowan Method
pc	2673.54	kPa	Joback Method
rinpol	1818.00		NIST Webbook
rinpol	1818.00		NIST Webbook
tb	652.17	K	Joback Method
tc	889.17	K	Joback Method
tf	382.89	K	Joback Method
vc	0.655	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	395.66	J/mol×K	652.17	Joback Method
cpg	408.68	J/mol×K	691.67	Joback Method
cpg	420.80	J/mol×K	731.17	Joback Method
cpg	432.04	J/mol×K	770.67	Joback Method
cpg	442.45	J/mol×K	810.17	Joback Method
cpg	452.06	J/mol×K	849.67	Joback Method
cpg	460.91	J/mol×K	889.17	Joback Method
dvisc	0.0016864	Pa×s	382.89	Joback Method

dvisc	0.0009611	Pa×s	427.77	Joback Method
dvisc	0.0006095	Pa×s	472.65	Joback Method
dvisc	0.0004182	Pa×s	517.53	Joback Method
dvisc	0.0003048	Pa×s	562.41	Joback Method
dvisc	0.0002328	Pa×s	607.29	Joback Method
dvisc	0.0001845	Pa×s	652.17	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U372932&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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