Phthalic acid, hexyl 3-iodobenzyl ester

Inchi: InChI=1S/C21H23IO4/c1-2-3-4-7-13-25-20(23)18-11-5-6-12-19(18)21(24)26-15-16-9-8-1
InchiKey: IMOGGKVXUVTHBO-UHFFFAOYSA-N
Formula: C21H23IO4
SMILES: CCCCCCOC(=O)c1ccccc1C(=O)OCc1cccc(I)c1
Mol. weight [g/mol]: 466.31

Physical Properties

Property code	Value	Unit	Source
gf	-78.22	kJ/mol	Joback Method
hf	-439.38	kJ/mol	Joback Method
hfus	47.43	kJ/mol	Joback Method
hvap	95.90	kJ/mol	Joback Method
log10ws	-7.31		Crippen Method
logp	5.385		Crippen Method
mcvol	299.930	ml/mol	McGowan Method
pc	1559.81	kPa	Joback Method
rinpol	3105.00		NIST Webbook
rinpol	3105.00		NIST Webbook
tb	988.92	K	Joback Method
tc	1230.92	K	Joback Method
tf	606.69	K	Joback Method
vc	1.131	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	880.47	J/mol×K	988.92	Joback Method
cpg	926.51	J/mol×K	1190.59	Joback Method
cpg	919.66	J/mol×K	1150.26	Joback Method
cpg	911.70	J/mol×K	1109.92	Joback Method
cpg	902.55	J/mol×K	1069.59	Joback Method
cpg	892.16	J/mol×K	1029.25	Joback Method
cpg	932.31	J/mol×K	1230.92	Joback Method
dvisc	0.0000353	Pa×s	988.92	Joback Method

dvisc	0.0000445	Pa×s	925.21	Joback Method
dvisc	0.0000582	Pa×s	861.51	Joback Method
dvisc	0.0000793	Pa×s	797.81	Joback Method
dvisc	0.0001141	Pa×s	734.10	Joback Method
dvisc	0.0001758	Pa×s	670.39	Joback Method
dvisc	0.0002969	Pa×s	606.69	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U378070&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
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