Phthalic acid, 3-iodobenzyl pentyl ester

Inchi: InChI=1S/C20H21IO4/c1-2-3-6-12-24-19(22)17-10-4-5-11-18(17)20(23)25-14-15-8-7-9-1
InchiKey: HXXSOVQWWFYROI-UHFFFAOYSA-N
Formula: C20H21IO4
SMILES: CCCCCOC(=O)c1ccccc1C(=O)OCc1cccc(I)c1
Mol. weight [g/mol]: 452.28

Physical Properties

Property code	Value	Unit	Source
gf	-86.64	kJ/mol	Joback Method
hf	-418.74	kJ/mol	Joback Method
hfus	44.84	kJ/mol	Joback Method
hvap	93.67	kJ/mol	Joback Method
log10ws	-6.89		Crippen Method
logp	4.995		Crippen Method
mcvol	285.840	ml/mol	McGowan Method
pc	1685.18	kPa	Joback Method
rinpol	2904.00		NIST Webbook
tb	966.04	K	Joback Method
tc	1209.57	K	Joback Method
tf	595.42	K	Joback Method
vc	1.075	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	822.42	J/mol×K	966.04	Joback Method
cpg	834.03	J/mol×K	1006.63	Joback Method
cpg	844.36	J/mol×K	1047.22	Joback Method
cpg	853.45	J/mol×K	1087.81	Joback Method
cpg	861.37	J/mol×K	1128.40	Joback Method
cpg	868.17	J/mol×K	1168.98	Joback Method
cpg	873.90	J/mol×K	1209.57	Joback Method
dvisc	0.0003330	Pa×s	595.42	Joback Method
dvisc	0.0001993	Pa×s	657.19	Joback Method

dvisc	0.0001303	Pa×s	718.96	Joback Method
dvisc	0.0000912	Pa×s	780.73	Joback Method
dvisc	0.0000672	Pa×s	842.50	Joback Method
dvisc	0.0000516	Pa×s	904.27	Joback Method
dvisc	0.0000410	Pa×s	966.04	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U378069&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