

Phthalic acid, 3-iodobenzyl isobutyl ester

Inchi:	InChI=1S/C19H19IO4/c1-13(2)11-23-18(21)16-8-3-4-9-17(16)19(22)24-12-14-6-5-7-15(2)
InchiKey:	PFSVTGBADPYZBZ-UHFFFAOYSA-N
Formula:	C19H19IO4
SMILES:	CC(C)COC(=O)c1ccccc1C(=O)OCc1cccc(I)c1
Mol. weight [g/mol]:	438.26

Physical Properties

Property code	Value	Unit	Source
gf	-97.50	kJ/mol	Joback Method
hf	-403.38	kJ/mol	Joback Method
hfus	38.73	kJ/mol	Joback Method
hvap	91.06	kJ/mol	Joback Method
log10ws	-6.23		Crippen Method
logp	4.461		Crippen Method
mvol	271.750	ml/mol	McGowan Method
pc	1838.84	kPa	Joback Method
rinpol	2758.00		NIST Webbook
rinpol	2758.00		NIST Webbook
tb	942.72	K	Joback Method
tc	1191.93	K	Joback Method
tf	569.15	K	Joback Method
vc	1.014	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	765.50	J/molxK	942.72	Joback Method
cpg	777.12	J/molxK	984.26	Joback Method
cpg	787.40	J/molxK	1025.79	Joback Method
cpg	796.41	J/molxK	1067.33	Joback Method
cpg	804.20	J/molxK	1108.86	Joback Method
cpg	810.82	J/molxK	1150.40	Joback Method
cpg	816.33	J/molxK	1191.93	Joback Method
dvisc	0.0004012	Paxs	569.15	Joback Method

dvisc	0.0002307	Paxs	631.41	Joback Method
dvisc	0.0001465	Paxs	693.67	Joback Method
dvisc	0.0001003	Paxs	755.94	Joback Method
dvisc	0.0000727	Paxs	818.20	Joback Method
dvisc	0.0000552	Paxs	880.46	Joback Method
dvisc	0.0000434	Paxs	942.72	Joback Method

Sources

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=U378067&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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