

Phthalic acid, 3-iodobenzyl propyl ester

Inchi:	InChI=1S/C18H17IO4/c1-2-10-22-17(20)15-8-3-4-9-16(15)18(21)23-12-13-6-5-7-14(19)1
InchiKey:	WMWIJCYNFSFMNEJ-UHFFFAOYSA-N
Formula:	C18H17IO4
SMILES:	CCCOC(=O)c1ccccc1C(=O)OCc1cccc(I)c1
Mol. weight [g/mol]:	424.23

Physical Properties

Property code	Value	Unit	Source
gf	-103.48	kJ/mol	Joback Method
hf	-377.46	kJ/mol	Joback Method
hfus	39.66	kJ/mol	Joback Method
hvap	89.22	kJ/mol	Joback Method
log10ws	-6.05		Crippen Method
logp	4.215		Crippen Method
mcvol	257.660	ml/mol	McGowan Method
pc	1985.89	kPa	Joback Method
rinqol	2709.00		NIST Webbook
tb	920.28	K	Joback Method
tc	1169.28	K	Joback Method
tf	572.88	K	Joback Method
vc	0.964	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	708.27	J/molxK	920.28	Joback Method
cpg	719.67	J/molxK	961.78	Joback Method
cpg	729.80	J/molxK	1003.28	Joback Method
cpg	738.70	J/molxK	1044.78	Joback Method
cpg	746.43	J/molxK	1086.28	Joback Method
cpg	753.04	J/molxK	1127.78	Joback Method
cpg	758.57	J/molxK	1169.28	Joback Method
dvisc	0.0004149	Paxs	572.88	Joback Method
dvisc	0.0002540	Paxs	630.78	Joback Method

dvisc	0.0001689	Paxs	688.68	Joback Method
dvisc	0.0001197	Paxs	746.58	Joback Method
dvisc	0.0000891	Paxs	804.48	Joback Method
dvisc	0.0000690	Paxs	862.38	Joback Method
dvisc	0.0000552	Paxs	920.28	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U378066&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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