

Phthalic acid, 3-iodobenzyl octyl ester

Inchi:	InChI=1S/C23H27IO4/c1-2-3-4-5-6-9-15-27-22(25)20-13-7-8-14-21(20)23(26)28-17-18-1
InchiKey:	YMGSHGRSWZRMSZ-UHFFFAOYSA-N
Formula:	C23H27IO4
SMILES:	CCCCCCCCOC(=O)c1cccc1C(=O)OCc1cccc(I)c1
Mol. weight [g/mol]:	494.36

Physical Properties

Property code	Value	Unit	Source
gf	-61.38	kJ/mol	Joback Method
hf	-480.66	kJ/mol	Joback Method
hfus	52.61	kJ/mol	Joback Method
hvap	100.35	kJ/mol	Joback Method
log10ws	-8.14		Crippen Method
logp	6.165		Crippen Method
mcvol	328.110	ml/mol	McGowan Method
pc	1347.68	kPa	Joback Method
rinsol	3205.00		NIST Webbook
tb	1034.68	K	Joback Method
tc	1276.24	K	Joback Method
tf	629.23	K	Joback Method
vc	1.244	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	998.29	J/molxK	1034.68	Joback Method
cpg	1010.10	J/molxK	1074.94	Joback Method
cpg	1020.57	J/molxK	1115.20	Joback Method
cpg	1029.79	J/molxK	1155.46	Joback Method
cpg	1037.81	J/molxK	1195.72	Joback Method
cpg	1044.71	J/molxK	1235.98	Joback Method
cpg	1050.55	J/molxK	1276.24	Joback Method
dvisc	0.0002341	Paxs	629.23	Joback Method
dvisc	0.0001358	Paxs	696.80	Joback Method

dvisc	0.0000868	Paxs	764.38	Joback Method
dvisc	0.0000596	Paxs	831.95	Joback Method
dvisc	0.0000433	Paxs	899.53	Joback Method
dvisc	0.0000329	Paxs	967.10	Joback Method
dvisc	0.0000259	Paxs	1034.68	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U378072&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

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