

Phthalic acid, 3-iodobenzyl nonyl ester

Inchi:	InChI=1S/C24H29IO4/c1-2-3-4-5-6-7-10-16-28-23(26)21-14-8-9-15-22(21)24(27)29-18-1
InchiKey:	VDGYITKUJVZWRJ-UHFFFAOYSA-N
Formula:	C24H29IO4
SMILES:	CCCCCCCCCOC(=O)c1ccccc1C(=O)OCc1cccc(I)c1
Mol. weight [g/mol]:	508.39

Physical Properties

Property code	Value	Unit	Source
gf	-52.96	kJ/mol	Joback Method
hf	-501.30	kJ/mol	Joback Method
hfus	55.20	kJ/mol	Joback Method
hvap	102.58	kJ/mol	Joback Method
log10ws	-8.56		Crippen Method
logp	6.556		Crippen Method
mcvol	342.200	ml/mol	McGowan Method
pc	1257.48	kPa	Joback Method
rinsol	3307.00		NIST Webbook
tb	1057.56	K	Joback Method
tc	1300.31	K	Joback Method
tf	640.50	K	Joback Method
vc	1.300	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1057.96	J/molxK	1057.56	Joback Method
cpg	1069.83	J/molxK	1098.02	Joback Method
cpg	1080.35	J/molxK	1138.48	Joback Method
cpg	1089.58	J/molxK	1178.94	Joback Method
cpg	1097.62	J/molxK	1219.39	Joback Method
cpg	1104.52	J/molxK	1259.85	Joback Method
cpg	1110.37	J/molxK	1300.31	Joback Method
dvisc	0.0002070	Paxs	640.50	Joback Method
dvisc	0.0001189	Paxs	710.01	Joback Method

dvisc	0.0000754	Paxs	779.52	Joback Method
dvisc	0.0000515	Paxs	849.03	Joback Method
dvisc	0.0000373	Paxs	918.54	Joback Method
dvisc	0.0000283	Paxs	988.05	Joback Method
dvisc	0.0000222	Paxs	1057.56	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=U378073&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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