Phthalic acid, decyl 3-iodobenzyl ester

Inchi: InChI=1S/C25H31IO4/c1-2-3-4-5-6-7-8-11-17-29-24(27)22-15-9-10-16-23(22)25(28)30-1
InchiKey: LNJPTELGHRUXQH-UHFFFAOYSA-N
Formula: C25H31IO4
SMILES: CCCCCCCCCCOC(=O)c1ccccc1C(=O)OCc1cccc(I)c1
Mol. weight [g/mol]: 522.42

Physical Properties

Property code	Value	Unit	Source
gf	-44.54	kJ/mol	Joback Method
hf	-521.94	kJ/mol	Joback Method
hfus	57.79	kJ/mol	Joback Method
hvap	104.81	kJ/mol	Joback Method
log10ws	-8.98		Crippen Method
logp	6.946		Crippen Method
mcvol	356.290	ml/mol	McGowan Method
pc	1176.05	kPa	Joback Method
rinpol	3408.00		NIST Webbook
rinpol	3408.00		NIST Webbook
tb	1080.44	K	Joback Method
tc	1325.38	K	Joback Method
tf	651.77	K	Joback Method
vc	1.355	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1118.08	J/mol×K	1080.44	Joback Method
cpg	1130.02	J/mol×K	1121.26	Joback Method
cpg	1140.59	J/mol×K	1162.09	Joback Method
cpg	1149.85	J/mol×K	1202.91	Joback Method
cpg	1157.89	J/mol×K	1243.74	Joback Method
cpg	1164.80	J/mol×K	1284.56	Joback Method
cpg	1170.65	J/mol×K	1325.38	Joback Method
dvisc	0.0001827	Pa×s	651.77	Joback Method

dvisc	0.0001039	Pa×s	723.22	Joback Method
dvisc	0.0000654	Pa×s	794.66	Joback Method
dvisc	0.0000445	Pa×s	866.11	Joback Method
dvisc	0.0000321	Pa×s	937.55	Joback Method
dvisc	0.0000242	Pa×s	1009.00	Joback Method
dvisc	0.0000190	Pa×s	1080.44	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=U378074&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