

Phthalic acid, dodecyl 3-iodobenzyl ester

Inchi:	InChI=1S/C27H35IO4/c1-2-3-4-5-6-7-8-9-10-13-19-31-26(29)24-17-11-12-18-25(24)27(3
InchiKey:	MADRXMPVBYPPEK-UHFFFAOYSA-N
Formula:	C27H35IO4
SMILES:	CCCCCCCCCCCCOC(=O)c1ccccc1C(=O)OCc1cccc(I)c1
Mol. weight [g/mol]:	550.47

Physical Properties

Property code	Value	Unit	Source
gf	-27.70	kJ/mol	Joback Method
hf	-563.22	kJ/mol	Joback Method
hfus	62.97	kJ/mol	Joback Method
hvap	109.26	kJ/mol	Joback Method
log10ws	-9.82		Crippen Method
logp	7.726		Crippen Method
mcvol	384.470	ml/mol	McGowan Method
pc	1035.23	kPa	Joback Method
rinsol	3604.00		NIST Webbook
tb	1126.20	K	Joback Method
tc	1378.79	K	Joback Method
tf	674.31	K	Joback Method
vc	1.468	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1239.54	J/molxK	1126.20	Joback Method
cpg	1251.69	J/molxK	1168.30	Joback Method
cpg	1262.38	J/molxK	1210.40	Joback Method
cpg	1271.71	J/molxK	1252.50	Joback Method
cpg	1279.78	J/molxK	1294.60	Joback Method
cpg	1286.69	J/molxK	1336.70	Joback Method
cpg	1292.54	J/molxK	1378.79	Joback Method
dvisc	0.0001412	Paxs	674.31	Joback Method
dvisc	0.0000789	Paxs	749.62	Joback Method

dvisc	0.0000490	Paxs	824.94	Joback Method
dvisc	0.0000330	Paxs	900.26	Joback Method
dvisc	0.0000236	Paxs	975.57	Joback Method
dvisc	0.0000177	Paxs	1050.88	Joback Method
dvisc	0.0000138	Paxs	1126.20	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=U378076&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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