

Phthalic acid, 3-iodobenzyl tridecyl ester

Inchi:	InChI=1S/C28H37IO4/c1-2-3-4-5-6-7-8-9-10-11-14-20-32-27(30)25-18-12-13-19-26(25)2
InchiKey:	QUMFNHMGDIUCPY-UHFFFAOYSA-N
Formula:	C28H37IO4
SMILES:	CCCCCCCCCCCCOC(=O)c1ccccc1C(=O)OCc1cccc(I)c1
Mol. weight [g/mol]:	564.50

Physical Properties

Property code	Value	Unit	Source
gf	-19.28	kJ/mol	Joback Method
hf	-583.86	kJ/mol	Joback Method
hfus	65.56	kJ/mol	Joback Method
hvap	111.48	kJ/mol	Joback Method
log10ws	-10.24		Crippen Method
logp	8.116		Crippen Method
mcvol	398.560	ml/mol	McGowan Method
pc	974.13	kPa	Joback Method
rinpol	3706.00		NIST Webbook
tb	1149.08	K	Joback Method
tc	1407.27	K	Joback Method
tf	685.58	K	Joback Method
vc	1.524	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1300.81	J/molxK	1149.08	Joback Method
cpg	1313.10	J/molxK	1192.11	Joback Method
cpg	1323.88	J/molxK	1235.14	Joback Method
cpg	1333.27	J/molxK	1278.17	Joback Method
cpg	1341.37	J/molxK	1321.20	Joback Method
cpg	1348.30	J/molxK	1364.23	Joback Method
cpg	1354.16	J/molxK	1407.27	Joback Method
dvisc	0.0001238	Paxs	685.58	Joback Method
dvisc	0.0000685	Paxs	762.83	Joback Method

dvisc	0.0000423	Paxs	840.08	Joback Method
dvisc	0.0000283	Paxs	917.33	Joback Method
dvisc	0.0000202	Paxs	994.58	Joback Method
dvisc	0.0000151	Paxs	1071.83	Joback Method
dvisc	0.0000117	Paxs	1149.08	Joback Method

Sources

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=U378077&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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