Isophthalic acid, octyl 3-phenylpropyl ester

Inchi: InChI=1S/C25H32O4/c1-2-3-4-5-6-10-18-28-24(26)22-16-11-17-23(20-22)25(27)29-19-1
InchiKey: XHGGUJXDCSYPJS-UHFFFAOYSA-N
Formula: C25H32O4
SMILES: CCCCCCCCOC(=O)c1cccc(C(=O)OCCCc2ccccc2)c1
Mol. weight [g/mol]: 396.52

Physical Properties

Property code	Value	Unit	Source
gf	-93.03	kJ/mol	Joback Method
hf	-587.34	kJ/mol	Joback Method
hfus	53.77	kJ/mol	Joback Method
hvap	94.77	kJ/mol	Joback Method
log10ws	-7.34		Crippen Method
logp	5.993		Crippen Method
mcvol	330.470	ml/mol	McGowan Method
pc	1206.47	kPa	Joback Method
rinpol	3217.00		NIST Webbook
tb	982.32	K	Joback Method
tc	1206.80	K	Joback Method
tf	581.19	K	Joback Method
vc	1.268	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1077.01	J/mol×K	982.32	Joback Method
cpg	1135.97	J/mol×K	1169.39	Joback Method
cpg	1126.79	J/mol×K	1131.97	Joback Method
cpg	1116.35	J/mol×K	1094.56	Joback Method
cpg	1104.62	J/mol×K	1057.15	Joback Method
cpg	1091.53	J/mol×K	1019.73	Joback Method
cpg	1143.97	J/mol×K	1206.80	Joback Method
dvisc	0.0000274	Pa×s	982.32	Joback Method
dvisc	0.0000354	Pa×s	915.46	Joback Method

dvisc	0.0000474	Pa×s	848.61	Joback Method
dvisc	0.0000669	Pa×s	781.75	Joback Method
dvisc	0.0001007	Pa×s	714.90	Joback Method
dvisc	0.0001649	Pa×s	648.05	Joback Method
dvisc	0.0003024	Pa×s	581.19	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344390&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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