Isophthalic acid, octyl 1-phenylpropyl ester

Inchi: InChI=1S/C25H32O4/c1-3-5-6-7-8-12-18-28-24(26)21-16-13-17-22(19-21)25(27)29-23(4
InchiKey: OOWOVZVATJLYLP-UHFFFAOYSA-N
Formula: C25H32O4
SMILES: CCCCCCCCOC(=O)c1cccc(C(=O)OC(CC)c2ccccc2)c1
Mol. weight [g/mol]: 396.52

Physical Properties

Property code	Value	Unit	Source
gf	-95.47	kJ/mol	Joback Method
hf	-592.62	kJ/mol	Joback Method
hfus	50.25	kJ/mol	Joback Method
hvap	94.38	kJ/mol	Joback Method
log10ws	-7.80		Crippen Method
logp	6.512		Crippen Method
mcvol	330.470	ml/mol	McGowan Method
pc	1213.20	kPa	Joback Method
rinpol	3061.00		NIST Webbook
rinpol	3061.00		NIST Webbook
tb	981.88	K	Joback Method
tc	1207.49	K	Joback Method
tf	566.19	K	Joback Method
vc	1.262	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1077.40	J/mol×K	981.88	Joback Method
cpg	1091.93	J/mol×K	1019.48	Joback Method
cpg	1105.01	J/mol×K	1057.08	Joback Method
cpg	1116.70	J/mol×K	1094.68	Joback Method
cpg	1127.06	J/mol×K	1132.29	Joback Method
cpg	1136.15	J/mol×K	1169.89	Joback Method
cpg	1144.02	J/mol×K	1207.49	Joback Method
dvisc	0.0003304	Pa×s	566.19	Joback Method

dvisc	0.0001699	Pa×s	635.47	Joback Method
dvisc	0.0000996	Pa×s	704.75	Joback Method
dvisc	0.0000642	Pa×s	774.03	Joback Method
dvisc	0.0000445	Pa×s	843.32	Joback Method
dvisc	0.0000326	Pa×s	912.60	Joback Method
dvisc	0.0000250	Pa×s	981.88	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344554&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

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