Isophthalic acid, 2-isopropylphenyl octyl ester

Inchi: InChI=1S/C25H32O4/c1-4-5-6-7-8-11-17-28-24(26)20-13-12-14-21(18-20)25(27)29-23-1
InchiKey: QCPMGXXCYKGWLZ-UHFFFAOYSA-N
Formula: C25H32O4
SMILES: CCCCCCCCOC(=O)c1cccc(C(=O)Oc2ccccc2C(C)C)c1
Mol. weight [g/mol]: 396.52

Physical Properties

Property code	Value	Unit	Source
gf	-105.10	kJ/mol	Joback Method
hf	-604.09	kJ/mol	Joback Method
hfus	49.86	kJ/mol	Joback Method
hvap	95.04	kJ/mol	Joback Method
log10ws	-7.92		Crippen Method
logp	6.546		Crippen Method
mcvol	330.470	ml/mol	McGowan Method
pc	1200.62	kPa	Joback Method
rinpol	3031.00		NIST Webbook
rinpol	3031.00		NIST Webbook
tb	986.86	K	Joback Method
tc	1213.38	K	Joback Method
tf	578.71	K	Joback Method
vc	1.262	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1076.37	J/mol×K	986.86	Joback Method
cpg	1134.00	J/mol×K	1175.63	Joback Method
cpg	1125.22	J/mol×K	1137.87	Joback Method
cpg	1115.13	J/mol×K	1100.12	Joback Method
cpg	1103.65	J/mol×K	1062.37	Joback Method
cpg	1090.75	J/mol×K	1024.61	Joback Method
cpg	1141.50	J/mol×K	1213.38	Joback Method
dvisc	0.0000256	Pa×s	986.86	Joback Method

dvisc	0.0000330	Pa×s	918.84	Joback Method
dvisc	0.0000444	Pa×s	850.81	Joback Method
dvisc	0.0000628	Pa×s	782.79	Joback Method
dvisc	0.0000951	Pa×s	714.76	Joback Method
dvisc	0.0001568	Pa×s	646.74	Joback Method
dvisc	0.0002911	Pa×s	578.71	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344638&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