Isophthalic acid, 4-isopropylphenyl nonyl ester

Inchi: InChI=1S/C26H34O4/c1-4-5-6-7-8-9-10-18-29-25(27)22-12-11-13-23(19-22)26(28)30-24
InchiKey: MCOKYPUIUFICII-UHFFFAOYSA-N
Formula: C26H34O4
SMILES: CCCCCCCCCOC(=O)c1cccc(C(=O)Oc2ccc(C(C)C)cc2)c1
Mol. weight [g/mol]: 410.55

Physical Properties

Property code	Value	Unit	Source
gf	-96.68	kJ/mol	Joback Method
hf	-624.73	kJ/mol	Joback Method
hfus	52.45	kJ/mol	Joback Method
hvap	97.27	kJ/mol	Joback Method
log10ws	-8.33		Crippen Method
logp	6.937		Crippen Method
mcvol	344.560	ml/mol	McGowan Method
pc	1124.57	kPa	Joback Method
rinpol	3312.00		NIST Webbook
rinpol	3312.00		NIST Webbook
tb	1009.74	K	Joback Method
tc	1238.66	K	Joback Method
tf	589.98	K	Joback Method
vc	1.317	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1137.07	J/mol×K	1009.74	Joback Method
cpg	1151.47	J/mol×K	1047.89	Joback Method
cpg	1164.36	J/mol×K	1086.05	Joback Method
cpg	1175.77	J/mol×K	1124.20	Joback Method
cpg	1185.76	J/mol×K	1162.35	Joback Method
cpg	1194.41	J/mol×K	1200.50	Joback Method
cpg	1201.75	J/mol×K	1238.66	Joback Method
dvisc	0.0002590	Pa×s	589.98	Joback Method

dvisc	0.0001382	Pa×s	659.94	Joback Method
dvisc	0.0000831	Pa×s	729.90	Joback Method
dvisc	0.0000547	Pa×s	799.86	Joback Method
dvisc	0.0000385	Pa×s	869.82	Joback Method
dvisc	0.0000285	Pa×s	939.78	Joback Method
dvisc	0.0000220	Pa×s	1009.74	Joback Method

Sources

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=U344460&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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