

Isophthalic acid, 2-isopropoxyphenyl nonyl ester

Inchi:	InChI=1S/C26H34O5/c1-4-5-6-7-8-9-12-18-29-25(27)21-14-13-15-22(19-21)26(28)31-24
InchiKey:	VTRWEFPEXDTZIN-UHFFFAOYSA-N
Formula:	C26H34O5
SMILES:	CCCCCCCCCOC(=O)c1cccc(C(=O)Oc2ccccc2OC(C)C)c1
Mol. weight [g/mol]:	426.55

Physical Properties

Property code	Value	Unit	Source
gf	-201.68	kJ/mol	Joback Method
hf	-756.95	kJ/mol	Joback Method
hfus	53.64	kJ/mol	Joback Method
hvap	99.68	kJ/mol	Joback Method
log10ws	-8.22		Crippen Method
logp	6.600		Crippen Method
mvol	350.430	ml/mol	McGowan Method
pc	1111.85	kPa	Joback Method
rinpol	3216.00		NIST Webbook
rinpol	3216.00		NIST Webbook
tb	1032.16	K	Joback Method
tc	1264.50	K	Joback Method
tf	612.21	K	Joback Method
vc	1.335	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1163.99	J/molxK	1032.16	Joback Method
cpg	1213.30	J/molxK	1225.78	Joback Method
cpg	1206.74	J/molxK	1187.05	Joback Method
cpg	1198.57	J/molxK	1148.33	Joback Method
cpg	1188.74	J/molxK	1109.61	Joback Method
cpg	1177.23	J/molxK	1070.88	Joback Method
cpg	1218.29	J/molxK	1264.50	Joback Method
dvisc	0.0000162	Paxs	1032.16	Joback Method

dvisc	0.0000210	Paxs	962.17	Joback Method
dvisc	0.0000282	Paxs	892.18	Joback Method
dvisc	0.0000398	Paxs	822.18	Joback Method
dvisc	0.0000599	Paxs	752.19	Joback Method
dvisc	0.0000982	Paxs	682.20	Joback Method
dvisc	0.0001801	Paxs	612.21	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344434&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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