

Isophthalic acid, nonyl 3-phenylpropyl ester

Inchi:	InChI=1S/C26H34O4/c1-2-3-4-5-6-7-11-19-29-25(27)23-17-12-18-24(21-23)26(28)30-20
InchiKey:	YXZZKKPQVNFBEU-UHFFFAOYSA-N
Formula:	C26H34O4
SMILES:	CCCCCCCCCOC(=O)c1cccc(C(=O)OCCc2ccccc2)c1
Mol. weight [g/mol]:	410.55

Physical Properties

Property code	Value	Unit	Source
gf	-84.61	kJ/mol	Joback Method
hf	-607.98	kJ/mol	Joback Method
hfus	56.36	kJ/mol	Joback Method
hvap	97.00	kJ/mol	Joback Method
log10ws	-7.76		Crippen Method
logp	6.384		Crippen Method
mvol	344.560	ml/mol	McGowan Method
pc	1129.86	kPa	Joback Method
rinpol	3322.00		NIST Webbook
rinpol	3322.00		NIST Webbook
tb	1005.20	K	Joback Method
tc	1232.41	K	Joback Method
tf	592.46	K	Joback Method
vc	1.323	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1137.76	J/molxK	1005.20	Joback Method
cpg	1196.71	J/molxK	1194.54	Joback Method
cpg	1187.59	J/molxK	1156.67	Joback Method
cpg	1177.21	J/molxK	1118.81	Joback Method
cpg	1165.48	J/molxK	1080.94	Joback Method
cpg	1152.36	J/molxK	1043.07	Joback Method
cpg	1204.61	J/molxK	1232.41	Joback Method
dvisc	0.0000236	Paxs	1005.20	Joback Method

dvisc	0.0000305	Paxs	936.41	Joback Method
dvisc	0.0000411	Paxs	867.62	Joback Method
dvisc	0.0000582	Paxs	798.83	Joback Method
dvisc	0.0000881	Paxs	730.04	Joback Method
dvisc	0.0001452	Paxs	661.25	Joback Method
dvisc	0.0002690	Paxs	592.46	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344391&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

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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