

Isophthalic acid, nonyl phenylethyl ester

Inchi:	InChI=1S/C25H32O4/c1-2-3-4-5-6-7-11-18-28-24(26)22-15-12-16-23(20-22)25(27)29-19
InchiKey:	WXGVQELWVJWFEM-UHFFFAOYSA-N
Formula:	C25H32O4
SMILES:	CCCCCCCCCOC(=O)c1cccc(C(=O)OCCc2ccccc2)c1
Mol. weight [g/mol]:	396.52

Physical Properties

Property code	Value	Unit	Source
gf	-93.03	kJ/mol	Joback Method
hf	-587.34	kJ/mol	Joback Method
hfus	53.77	kJ/mol	Joback Method
hvap	94.77	kJ/mol	Joback Method
log10ws	-7.34		Crippen Method
logp	5.993		Crippen Method
mvol	330.470	ml/mol	McGowan Method
pc	1206.47	kPa	Joback Method
rinpol	3208.00		NIST Webbook
rinpol	3208.00		NIST Webbook
tb	982.32	K	Joback Method
tc	1206.80	K	Joback Method
tf	581.19	K	Joback Method
vc	1.268	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1077.01	J/molxK	982.32	Joback Method
cpg	1091.53	J/molxK	1019.73	Joback Method
cpg	1104.62	J/molxK	1057.15	Joback Method
cpg	1116.35	J/molxK	1094.56	Joback Method
cpg	1126.79	J/molxK	1131.97	Joback Method
cpg	1135.97	J/molxK	1169.39	Joback Method
cpg	1143.97	J/molxK	1206.80	Joback Method
dvisc	0.0003024	Paxs	581.19	Joback Method

dvisc	0.0001649	Paxs	648.05	Joback Method
dvisc	0.0001007	Paxs	714.90	Joback Method
dvisc	0.0000669	Paxs	781.75	Joback Method
dvisc	0.0000474	Paxs	848.61	Joback Method
dvisc	0.0000354	Paxs	915.46	Joback Method
dvisc	0.0000274	Paxs	982.32	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344340&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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