

Isophthalic acid, nonyl 1-propylbutyl ester

Inchi:	InChI=1S/C24H38O4/c1-4-7-8-9-10-11-12-18-27-23(25)20-16-13-17-21(19-20)24(26)28-
InchiKey:	NINNOANFPBBLHZ-UHFFFAOYSA-N
Formula:	C24H38O4
SMILES:	CCCCCCCCCOC(=O)c1cccc(C(=O)OC(CCC)CCC)c1
Mol. weight [g/mol]:	390.56

Physical Properties

Property code	Value	Unit	Source
gf	-216.30	kJ/mol	Joback Method
hf	-808.51	kJ/mol	Joback Method
hfus	53.62	kJ/mol	Joback Method
hvap	89.88	kJ/mol	Joback Method
log10ws	-7.93		Crippen Method
logp	6.720		Crippen Method
mcvol	340.140	ml/mol	McGowan Method
pc	1036.57	kPa	Joback Method
rinpol	2696.00		NIST Webbook
tb	932.32	K	Joback Method
tc	1142.37	K	Joback Method
tf	528.50	K	Joback Method
vc	1.313	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1119.86	J/molxK	932.32	Joback Method
cpg	1191.53	J/molxK	1107.36	Joback Method
cpg	1179.81	J/molxK	1072.35	Joback Method
cpg	1166.82	J/molxK	1037.34	Joback Method
cpg	1152.52	J/molxK	1002.34	Joback Method
cpg	1136.88	J/molxK	967.33	Joback Method
cpg	1202.02	J/molxK	1142.37	Joback Method
dvisc	0.0000281	Paxs	932.32	Joback Method
dvisc	0.0000371	Paxs	865.02	Joback Method

dvisc	0.0000513	Paxs	797.71	Joback Method
dvisc	0.0000753	Paxs	730.41	Joback Method
dvisc	0.0001196	Paxs	663.11	Joback Method
dvisc	0.0002108	Paxs	595.80	Joback Method
dvisc	0.0004292	Paxs	528.50	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356404&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
mccvol:	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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