

Isophthalic acid, nonyl phenyl ester

Inchi:	InChI=1S/C23H28O4/c1-2-3-4-5-6-7-11-17-26-22(24)19-13-12-14-20(18-19)23(25)27-21
InchiKey:	GLSPFVSSIZLOLL-UHFFFAOYSA-N
Formula:	C23H28O4
SMILES:	CCCCCCCCCOC(=O)c1cccc(C(=O)Oc2ccccc2)c1
Mol. weight [g/mol]:	368.47

Physical Properties

Property code	Value	Unit	Source
gf	-109.87	kJ/mol	Joback Method
hf	-546.06	kJ/mol	Joback Method
hfus	48.59	kJ/mol	Joback Method
hvap	90.32	kJ/mol	Joback Method
log10ws	-7.15		Crippen Method
logp	5.813		Crippen Method
mvol	302.290	ml/mol	McGowan Method
pc	1385.05	kPa	Joback Method
rinpol	3025.00		NIST Webbook
rinpol	3025.00		NIST Webbook
tb	936.56	K	Joback Method
tc	1158.33	K	Joback Method
tf	558.65	K	Joback Method
vc	1.155	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	957.00	J/molxK	936.56	Joback Method
cpg	971.39	J/molxK	973.52	Joback Method
cpg	984.43	J/molxK	1010.48	Joback Method
cpg	996.18	J/molxK	1047.44	Joback Method
cpg	1006.67	J/molxK	1084.41	Joback Method
cpg	1015.97	J/molxK	1121.37	Joback Method
cpg	1024.11	J/molxK	1158.33	Joback Method
dvisc	0.0003786	Paxs	558.65	Joback Method

dvisc	0.0002108	Paxs	621.63	Joback Method
dvisc	0.0001307	Paxs	684.62	Joback Method
dvisc	0.0000879	Paxs	747.61	Joback Method
dvisc	0.0000628	Paxs	810.59	Joback Method
dvisc	0.0000472	Paxs	873.57	Joback Method
dvisc	0.0000368	Paxs	936.56	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344362&Units=SI

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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