

Phthalic acid, 3-methoxy-4-nitrobenzyl nonyl ester

Inchi:	InChI=1S/C25H31NO7/c1-3-4-5-6-7-8-11-16-32-24(27)20-12-9-10-13-21(20)25(28)33-18
InchiKey:	HKIXTKBFWNLNQB-UHFFFAOYSA-N
Formula:	C25H31NO7
SMILES:	CCCCCCCCCOC(=O)c1ccccc1C(=O)OCc1ccc([N+](=O)[O-])c(OC)c1
Mol. weight [g/mol]:	457.52

Physical Properties

Property code	Value	Unit	Source
gf	-181.74	kJ/mol	Joback Method
hf	-753.26	kJ/mol	Joback Method
hfus	65.54	kJ/mol	Joback Method
hvap	115.09	kJ/mol	Joback Method
log10ws	-8.19		Crippen Method
logp	5.868		Crippen Method
mvol	353.760	ml/mol	McGowan Method
pc	1177.66	kPa	Joback Method
rinpol	3986.00		NIST Webbook
rinpol	3986.00		NIST Webbook
tb	1166.54	K	Joback Method
tc	1428.56	K	Joback Method
tf	772.07	K	Joback Method
vc	1.367	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1190.50	J/mol×K	1166.54	Joback Method
cpg	1197.81	J/mol×K	1210.21	Joback Method
cpg	1203.06	J/mol×K	1253.88	Joback Method
cpg	1206.29	J/mol×K	1297.55	Joback Method
cpg	1207.55	J/mol×K	1341.22	Joback Method
cpg	1206.89	J/mol×K	1384.89	Joback Method
cpg	1204.35	J/mol×K	1428.56	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=U382537&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/95-260-8/Phthalic-acid-3-methoxy-4-nitrobenzyl-nonyl-ester.pdf>

Generated by Cheméo on 2024-05-03 16:14:43.244661486 +0000 UTC m=+17042132.165238801.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.