

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

Inchi:	InChI=1S/C25H31NO6/c1-3-4-5-6-7-8-11-16-31-24(27)21-12-9-10-13-22(21)25(28)32-18
InchiKey:	ONUHFQHGMLQSG-UHFFFAOYSA-N
Formula:	C25H31NO6
SMILES:	CCCCCCCCCOC(=O)c1ccccc1C(=O)OCc1ccc(C)c([N+](=O)[O-])c1
Mol. weight [g/mol]:	441.52

Physical Properties

Property code	Value	Unit	Source
gf	-76.74	kJ/mol	Joback Method
hf	-621.04	kJ/mol	Joback Method
hfus	64.36	kJ/mol	Joback Method
hvap	112.69	kJ/mol	Joback Method
log10ws	-8.54		Crippen Method
logp	6.168		Crippen Method
mvol	347.890	ml/mol	McGowan Method
pc	1191.52	kPa	Joback Method
rinpol	3685.00		NIST Webbook
rinpol	3685.00		NIST Webbook
tb	1144.12	K	Joback Method
tc	1400.73	K	Joback Method
tf	749.84	K	Joback Method
vc	1.349	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1169.50	J/mol×K	1144.12	Joback Method
cpg	1178.94	J/mol×K	1186.89	Joback Method
cpg	1186.67	J/mol×K	1229.66	Joback Method
cpg	1192.77	J/mol×K	1272.43	Joback Method
cpg	1197.32	J/mol×K	1315.19	Joback Method
cpg	1200.38	J/mol×K	1357.96	Joback Method
cpg	1202.03	J/mol×K	1400.73	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=U382587&Units=SI

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

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