

Phthalic acid, 4-nitrobenzyl propyl ester

Inchi:	InChI=1S/C18H17NO6/c1-2-11-24-17(20)15-5-3-4-6-16(15)18(21)25-12-13-7-9-14(10-8-
InchiKey:	YYUQICONHZODBX-UHFFFAOYSA-N
Formula:	C18H17NO6
SMILES:	CCCOC(=O)c1ccccc1C(=O)OCc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]:	343.33

Physical Properties

Property code	Value	Unit	Source
gf	-126.05	kJ/mol	Joback Method
hf	-465.09	kJ/mol	Joback Method
hfus	46.61	kJ/mol	Joback Method
hvap	96.44	kJ/mol	Joback Method
log10ws	-5.55		Crippen Method
logp	3.519		Crippen Method
mvol	249.260	ml/mol	McGowan Method
pc	2047.46	kPa	Joback Method
rinpol	3140.00		NIST Webbook
rinpol	3140.00		NIST Webbook
tb	978.98	K	Joback Method
tc	1226.15	K	Joback Method
tf	658.43	K	Joback Method
vc	0.958	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	760.93	J/mol×K	978.98	Joback Method
cpg	770.73	J/mol×K	1020.17	Joback Method
cpg	779.14	J/mol×K	1061.37	Joback Method
cpg	786.21	J/mol×K	1102.56	Joback Method
cpg	791.98	J/mol×K	1143.76	Joback Method
cpg	796.49	J/mol×K	1184.95	Joback Method
cpg	799.77	J/mol×K	1226.15	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=U382520&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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