

p-Nitrophenyl hexadecyl ether

Inchi:	InChI=1S/C22H37NO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-20-26-22-18-16-21(17-19-
InchiKey:	HOBVESXNPYPANG-UHFFFAOYSA-N
Formula:	C22H37NO3
SMILES:	CCCCCCCCCCCCCCCCOc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]:	363.53
CAS:	102703-33-3

Physical Properties

Property code	Value	Unit	Source
gf	167.69	kJ/mol	Joback Method
hf	-415.33	kJ/mol	Joback Method
hfus	58.94	kJ/mol	Joback Method
hvap	86.50	kJ/mol	Joback Method
log10ws	-8.52		Crippen Method
logp	7.455		Crippen Method
mcvol	320.370	ml/mol	McGowan Method
pc	1097.17	kPa	Joback Method
tb	908.68	K	Joback Method
tc	1117.91	K	Joback Method
tf	542.48	K	Joback Method
vc	1.260	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1054.16	J/molxK	908.68	Joback Method
cpg	1071.67	J/molxK	943.55	Joback Method
cpg	1087.98	J/molxK	978.42	Joback Method
cpg	1103.15	J/molxK	1013.30	Joback Method
cpg	1117.22	J/molxK	1048.17	Joback Method
cpg	1130.27	J/molxK	1083.04	Joback Method
cpg	1142.34	J/molxK	1117.91	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C102703333&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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