

4-Nitrobenzoic acid, nonyl ester

Other names:	nonyl 4-nitrobenzoate
Inchi:	InChI=1S/C16H23NO4/c1-2-3-4-5-6-7-8-13-21-16(18)14-9-11-15(12-10-14)17(19)20/h9-
InchiKey:	VCWKTBZKTLGBGP-UHFFFAOYSA-N
Formula:	C16H23NO4
SMILES:	CCCCCCCCCOC(=O)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]:	293.36
CAS:	6500-27-2

Physical Properties

Property code	Value	Unit	Source
gf	-11.75	kJ/mol	Joback Method
hf	-404.07	kJ/mol	Joback Method
hfus	45.00	kJ/mol	Joback Method
hvap	79.89	kJ/mol	Joback Method
log10ws	-5.71		Crippen Method
logp	4.502		Crippen Method
mcvol	237.400	ml/mol	McGowan Method
pc	1765.41	kPa	Joback Method
ripol	2227.00		NIST Webbook
ripol	2208.00		NIST Webbook
ripol	2220.00		NIST Webbook
ripol	2232.00		NIST Webbook
ripol	2241.00		NIST Webbook
ripol	2200.00		NIST Webbook
ripol	2200.00		NIST Webbook
ripol	2227.00		NIST Webbook
ripol	2979.00		NIST Webbook
ripol	2979.00		NIST Webbook
ripol	3014.00		NIST Webbook
ripol	3029.00		NIST Webbook
ripol	3021.00		NIST Webbook
ripol	3021.00		NIST Webbook
tb	825.27	K	Joback Method
tc	1041.92	K	Joback Method
tf	524.79	K	Joback Method
vc	0.929	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	716.23	J/mol×K	825.27	Joback Method
cpg	730.76	J/mol×K	861.38	Joback Method
cpg	744.22	J/mol×K	897.49	Joback Method
cpg	756.65	J/mol×K	933.60	Joback Method
cpg	768.10	J/mol×K	969.71	Joback Method
cpg	778.60	J/mol×K	1005.82	Joback Method
cpg	788.18	J/mol×K	1041.92	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=C6500272&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
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume

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