4-Nitrobenzoic acid, heptyl ester

Other names: Benzoic acid, 4-nitro, heptyl ester
heptyl 4-nitrobenzoate
Inchi: InChI=1S/C14H19NO4/c1-2-3-4-5-6-11-19-14(16)12-7-9-13(10-8-12)15(17)18/h7-10H,2-
InchiKey: WMUVYRILEXKYQK-UHFFFAOYSA-N
Formula: C14H19NO4
SMILES: CCCCCCCOC(=O)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 265.31
CAS: 14309-44-5

Physical Properties

Property code	Value	Unit	Source
gf	-28.59	kJ/mol	Joback Method
hf	-362.79	kJ/mol	Joback Method
hfus	39.82	kJ/mol	Joback Method
hvap	75.44	kJ/mol	Joback Method
log10ws	-4.88		Crippen Method
logp	3.722		Crippen Method
mcvol	209.220	ml/mol	McGowan Method
pc	2088.84	kPa	Joback Method
rinpol	1999.00		NIST Webbook
rinpol	2007.00		NIST Webbook
rinpol	2018.00		NIST Webbook
rinpol	2031.00		NIST Webbook
rinpol	2039.00		NIST Webbook
rinpol	2016.00		NIST Webbook
rinpol	2007.00		NIST Webbook
rinpol	2039.00		NIST Webbook
rinpol	2016.00		NIST Webbook
rinpol	2007.00		NIST Webbook
ripol	2800.00		NIST Webbook
ripol	2800.00		NIST Webbook
ripol	2771.00		NIST Webbook
ripol	2771.00		NIST Webbook
ripol	2806.00		NIST Webbook
ripol	2824.00		NIST Webbook
tb	779.51	K	Joback Method
tc	1000.99	K	Joback Method

tf	502.25	K	Joback Method
vc	0.818	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	604.78	J/mol×K	779.51	Joback Method
cpg	618.77	J/mol×K	816.42	Joback Method
cpg	631.73	J/mol×K	853.34	Joback Method
cpg	643.71	J/mol×K	890.25	Joback Method
cpg	654.73	J/mol×K	927.16	Joback Method
cpg	664.82	J/mol×K	964.07	Joback Method
cpg	674.02	J/mol×K	1000.99	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C14309445&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
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