4-Nitrobenzoic acid, decyl ester

Other names: decyl 4-nitrobenzoate
Inchi: InChI=1S/C17H25NO4/c1-2-3-4-5-6-7-8-9-14-22-17(19)15-10-12-16(13-11-15)18(20)21/
InchiKey: XRQVVCKJAIGRHJ-UHFFFAOYSA-N
Formula: C17H25NO4
SMILES: CCCCCCCCCCOC(=O)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 307.38
CAS: 6500-30-7

Physical Properties

Property code	Value	Unit	Source
gf	-3.33	kJ/mol	Joback Method
hf	-424.71	kJ/mol	Joback Method
hfus	47.59	kJ/mol	Joback Method
hvap	82.12	kJ/mol	Joback Method
log10ws	-6.13		Crippen Method
logp	4.892		Crippen Method
mcvol	251.490	ml/mol	McGowan Method
pc	1631.17	kPa	Joback Method
rinpol	2333.00		NIST Webbook
rinpol	2299.00		NIST Webbook
rinpol	2308.00		NIST Webbook
rinpol	2321.00		NIST Webbook
rinpol	2333.00		NIST Webbook
rinpol	2342.00		NIST Webbook
rinpol	2333.00		NIST Webbook
rinpol	2299.00		NIST Webbook
ripol	3130.00		NIST Webbook
ripol	3131.00		NIST Webbook
ripol	3130.00		NIST Webbook
ripol	3082.00		NIST Webbook
ripol	3082.00		NIST Webbook
ripol	3117.00		NIST Webbook
tb	848.15	K	Joback Method
tc	1063.31	K	Joback Method
tf	536.06	K	Joback Method
vc	0.986	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	773.35	J/mol×K	848.15	Joback Method
cpg	788.10	J/mol×K	884.01	Joback Method
cpg	801.75	J/mol×K	919.87	Joback Method
cpg	814.37	J/mol×K	955.73	Joback Method
cpg	825.98	J/mol×K	991.59	Joback Method
cpg	836.62	J/mol×K	1027.45	Joback Method
cpg	846.35	J/mol×K	1063.31	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6500307&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

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