Dodecyl 4-nitrophenyl ether

Other names: p-Dodecyloxynitrobenzene
Inchi: InChI=1S/C18H29NO3/c1-2-3-4-5-6-7-8-9-10-11-16-22-18-14-12-17(13-15-18)19(20)21/
InchiKey: VZOAOBWVYOLSII-UHFFFAOYSA-N
Formula: C18H29NO3
SMILES: CCCCCCCCCCCCOc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 307.43
CAS: 65039-18-1

Physical Properties

Property code	Value	Unit	Source
gf	134.01	kJ/mol	Joback Method
hf	-332.77	kJ/mol	Joback Method
hfus	48.58	kJ/mol	Joback Method
hvap	77.60	kJ/mol	Joback Method
log10ws	-6.85		Crippen Method
logp	5.894		Crippen Method
mcvol	264.010	ml/mol	McGowan Method
pc	1440.25	kPa	Joback Method
tb	817.16	K	Joback Method
tc	1024.53	K	Joback Method
tf	497.40	K	Joback Method
vc	1.036	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	814.56	J/mol×K	817.16	Joback Method
cpg	831.27	J/mol×K	851.72	Joback Method
cpg	846.90	J/mol×K	886.28	Joback Method
cpg	861.47	J/mol×K	920.84	Joback Method
cpg	875.04	J/mol×K	955.41	Joback Method
cpg	887.65	J/mol×K	989.97	Joback Method
cpg	899.33	J/mol×K	1024.53	Joback Method

Sources

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=C65039181&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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