

Benzamide, 4-nitro-N-ethyl-N-tetradecyl-

Inchi:	InChI=1S/C23H38N2O3/c1-3-5-6-7-8-9-10-11-12-13-14-15-20-24(4-2)23(26)21-16-18-22
InchiKey:	JKDWHFVBDZETCS-UHFFFAOYSA-N
Formula:	C23H38N2O3
SMILES:	CCCCCCCCCCCCCN(CC)C(=O)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]:	390.56

Physical Properties

Property code	Value	Unit	Source
gf	262.97	kJ/mol	Joback Method
hf	-348.80	kJ/mol	Joback Method
hfus	64.96	kJ/mol	Joback Method
hvap	95.11	kJ/mol	Joback Method
log10ws	-8.13		Crippen Method
logp	6.758		Crippen Method
mvol	340.140	ml/mol	McGowan Method
pc	1084.20	kPa	Joback Method
rinpol	1610.00		NIST Webbook
rinpol	1610.00		NIST Webbook
tb	975.45	K	Joback Method
tc	1195.52	K	Joback Method
tf	613.92	K	Joback Method
vc	1.321	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1146.28	J/molxK	975.45	Joback Method
cpg	1163.05	J/molxK	1012.13	Joback Method
cpg	1178.69	J/molxK	1048.81	Joback Method
cpg	1193.30	J/molxK	1085.48	Joback Method
cpg	1206.97	J/molxK	1122.16	Joback Method
cpg	1219.79	J/molxK	1158.84	Joback Method
cpg	1231.85	J/molxK	1195.52	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415299&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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