Benzamide, 4-nitro-N-ethyl-N-hexadecyl-

Inchi: InChI=1S/C25H42N2O3/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-22-26(4-2)25(28)23-18
InchiKey: DVMRDQILQZUAPQ-UHFFFAOYSA-N
Formula: C25H42N2O3
SMILES: CCCCCCCCCCCCCCCCN(CC)C(=O)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 418.61

Physical Properties

Property code	Value	Unit	Source
gf	279.81	kJ/mol	Joback Method
hf	-390.08	kJ/mol	Joback Method
hfus	70.14	kJ/mol	Joback Method
hvap	99.56	kJ/mol	Joback Method
log10ws	-8.96		Crippen Method
logp	7.538		Crippen Method
mcvol	368.320	ml/mol	McGowan Method
pc	959.10	kPa	Joback Method
rinpol	1648.00		NIST Webbook
rinpol	1648.00		NIST Webbook
tb	1021.21	K	Joback Method
tc	1250.35	K	Joback Method
tf	636.46	K	Joback Method
vc	1.433	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1271.12	J/mol×K	1021.21	Joback Method
cpg	1288.67	J/mol×K	1059.40	Joback Method
cpg	1305.04	J/mol×K	1097.59	Joback Method
cpg	1320.32	J/mol×K	1135.78	Joback Method
cpg	1334.64	J/mol×K	1173.97	Joback Method
cpg	1348.11	J/mol×K	1212.16	Joback Method
cpg	1360.84	J/mol×K	1250.35	Joback Method

Sources

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=U415300&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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