Benzamide, 4-nitro-N-ethyl-N-heptyl-

Inchi: InChI=1S/C16H24N2O3/c1-3-5-6-7-8-13-17(4-2)16(19)14-9-11-15(12-10-14)18(20)21/h9
InchiKey: DOFZTWNLLZMBDH-UHFFFAOYSA-N
Formula: C16H24N2O3
SMILES: CCCCCCCN(CC)C(=O)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 292.37

Physical Properties

Property code	Value	Unit	Source
gf	204.03	kJ/mol	Joback Method
hf	-204.32	kJ/mol	Joback Method
hfus	46.83	kJ/mol	Joback Method
hvap	79.53	kJ/mol	Joback Method
log10ws	-5.20		Crippen Method
logp	4.027		Crippen Method
mcvol	241.510	ml/mol	McGowan Method
pc	1787.88	kPa	Joback Method
rinpol	2595.00		NIST Webbook
rinpol	2595.00		NIST Webbook
tb	815.29	K	Joback Method
tc	1031.28	K	Joback Method
tf	535.03	K	Joback Method
vc	0.929	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	729.72	J/mol×K	815.29	Joback Method
cpg	744.75	J/mol×K	851.29	Joback Method
cpg	758.73	J/mol×K	887.29	Joback Method
cpg	771.74	J/mol×K	923.28	Joback Method
cpg	783.83	J/mol×K	959.28	Joback Method
cpg	795.08	J/mol×K	995.28	Joback Method
cpg	805.55	J/mol×K	1031.28	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=U415293&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