Benzene, 1-nitro-3-(phenylmethyl)-

Other names: Methane, (m-nitrophenyl)phenyl-
m-Nitrodiphenylmethane
Inchi: InChI=1S/C13H11NO2/c15-14(16)13-8-4-7-12(10-13)9-11-5-2-1-3-6-11/h1-8,10H,9H2
InchiKey: CMTUCQNYLNHJRT-UHFFFAOYSA-N
Formula: C13H11NO2
SMILES: O=[N+]([O-])c1cccc(Cc2ccccc2)c1
Mol. weight [g/mol]: 213.23
CAS: 5840-41-5

Physical Properties

Property code	Value	Unit	Source
gf	309.32	kJ/mol	Joback Method
hf	139.18	kJ/mol	Joback Method
hfus	28.48	kJ/mol	Joback Method
hvap	66.34	kJ/mol	Joback Method
log10ws	-4.22		Crippen Method
logp	3.186		Crippen Method
mcvol	163.930	ml/mol	McGowan Method
pc	3062.55	kPa	Joback Method
rinpol	1858.70		NIST Webbook
rinpol	1858.70		NIST Webbook
rinpol	1898.00		NIST Webbook
tb	707.02	K	Joback Method
tc	975.37	K	Joback Method
tf	445.24	K	Joback Method
vc	0.629	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	423.97	J/mol×K	707.02	Joback Method
cpg	438.23	J/mol×K	751.74	Joback Method
cpg	451.16	J/mol×K	796.47	Joback Method
cpg	462.88	J/mol×K	841.19	Joback Method

cpg	473.48	J/mol×K	885.92	Joback Method
cpg	483.06	J/mol×K	930.64	Joback Method
cpg	491.73	J/mol×K	975.37	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=C5840415&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume