2-Nitro-2-methyl-3-phenyl-1-propanol

Inchi: InChI=1S/C10H13NO3/c1-10(8-12,11(13)14)7-9-5-3-2-4-6-9/h2-6,12H,7-8H2,1H3
InchiKey: PLKSTJNBJNDHOL-UHFFFAOYSA-N
Formula: C10H13NO3
SMILES: CC(CO)(Cc1ccccc1)[N+](=O)[O-]
Mol. weight [g/mol]: 195.22
CAS: 62030-36-8

Physical Properties

Property code	Value	Unit	Source
chs	-5445.40 ± 4.40	kJ/mol	NIST Webbook
chs	-5445.40 ± 4.40	kJ/mol	NIST Webbook
gf	47.30	kJ/mol	Joback Method
hf	-184.94	kJ/mol	Joback Method
hfs	-347.70 ± 4.40	kJ/mol	NIST Webbook
hfs	-347.70 ± 4.40	kJ/mol	NIST Webbook
hfus	23.73	kJ/mol	Joback Method
hvap	72.10	kJ/mol	Joback Method
log10ws	-2.57		Crippen Method
logp	1.257		Crippen Method
mcvol	151.290	ml/mol	McGowan Method
pc	3364.54	kPa	Joback Method
tb	695.67	K	Joback Method
tc	922.75	K	Joback Method
tf	435.73	K	Joback Method
vc	0.578	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	411.55	J/mol×K	695.67	Joback Method
cpg	423.08	J/mol×K	733.52	Joback Method
cpg	433.71	J/mol×K	771.36	Joback Method
cpg	443.52	J/mol×K	809.21	Joback Method
cpg	452.57	J/mol×K	847.06	Joback Method

cpg	460.95	J/mol×K	884.91	Joback Method
cpg	468.73	J/mol×K	922.75	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C62030368&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase 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