4-(p-Nitrophenyl)butyric acid

Other names:	4-(p-Nitrophenyl)butyric acid
	Benzenebutanoic acid, 4-nitro-
	«gamma»-(p-Nitrophenyl)butyric acid
Inchi:	InChI=1S/C10H11NO4/c12-10(13)3-1-2-8-4-6-9(7-5-8)11(14)15/h4-7H,1-3H2,(H,12,13)
InchiKey:	WQMLUHZFRFCQDB-UHFFFAOYSA-N
Formula:	C10H11NO4
SMILES:	O=C(O)CCCc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]:	209.20

Physical Properties

Property code	Value	Unit	Source
hf	-348.27	kJ/mol	Cheméo Relay (1.0)
hfus	32.36	kJ/mol	Joback Method
hvap	110.93	kJ/mol	Cheméo Relay (1.0)
ie	9.42	eV	Cheméo Relay (1.0)
log10ws	-2.70		Cheméo Relay (1.0)
logp	2.002		Crippen Method
mcvol	152.860	ml/mol	McGowan Method
pc	3480.65	kPa	Joback Method
tb	586.13	K	Cheméo Relay (1.0)
tf	364.39	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	416.30	J/mol×K	757.75	Joback Method
cpg	426.00	J/mol×K	794.78	Joback Method
cpg	434.98	J/mol×K	831.80	Joback Method
cpg	443.25	J/mol×K	868.83	Joback Method
cpg	450.88	J/mol×K	905.85	Joback Method
cpg	457.89	J/mol×K	942.88	Joback Method
cpg	464.33	J/mol×K	979.90	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5600624&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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
tf:	Normal melting (fusion) point