4-Bromobutyric acid, 4-nitrophenyl ester

Inchi: InChI=1S/C10H10BrNO4/c11-7-1-2-10(13)16-9-5-3-8(4-6-9)12(14)15/h3-6H,1-2,7H2
InchiKey: GAAZAZYRJDROIQ-UHFFFAOYSA-N
Formula: C10H10BrNO4
SMILES: O=C(CCCBr)Oc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 288.10

Physical Properties

Property code	Value	Unit	Source
gf	-47.95	kJ/mol	Joback Method
hf	-253.90	kJ/mol	Joback Method
hfus	34.74	kJ/mol	Joback Method
hvap	72.97	kJ/mol	Joback Method
log10ws	-3.70		Crippen Method
logp	2.675		Crippen Method
mcvol	170.360	ml/mol	McGowan Method
pc	3322.01	kPa	Joback Method
rinpol	2009.00		NIST Webbook
tb	754.15	K	Joback Method
tc	1001.53	K	Joback Method
tf	516.97	K	Joback Method
vc	0.655	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	425.95	J/mol×K	754.15	Joback Method
cpg	436.57	J/mol×K	795.38	Joback Method
cpg	446.26	J/mol×K	836.61	Joback Method
cpg	455.09	J/mol×K	877.84	Joback Method
cpg	463.08	J/mol×K	919.07	Joback Method
cpg	470.27	J/mol×K	960.30	Joback Method
cpg	476.72	J/mol×K	1001.53	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307612&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

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