5-Bromovaleric acid, 4-nitrophenyl ester

Inchi: InChI=1S/C11H12BrNO4/c12-8-2-1-3-11(14)17-10-6-4-9(5-7-10)13(15)16/h4-7H,1-3,8H2
InchiKey: GDGCLFKJKUESDK-UHFFFAOYSA-N
Formula: C11H12BrNO4
SMILES: O=C(CCCCBr)Oc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 302.12

Physical Properties

Property code	Value	Unit	Source
gf	-39.53	kJ/mol	Joback Method
hf	-274.54	kJ/mol	Joback Method
hfus	37.33	kJ/mol	Joback Method
hvap	75.20	kJ/mol	Joback Method
log10ws	-4.12		Crippen Method
logp	3.065		Crippen Method
mcvol	184.450	ml/mol	McGowan Method
pc	2982.79	kPa	Joback Method
rinpol	2143.00		NIST Webbook
tb	777.03	K	Joback Method
tc	1019.47	K	Joback Method
tf	528.24	K	Joback Method
vc	0.712	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	477.60	J/mol×K	777.03	Joback Method
cpg	488.76	J/mol×K	817.44	Joback Method
cpg	498.98	J/mol×K	857.84	Joback Method
cpg	508.30	J/mol×K	898.25	Joback Method
cpg	516.77	J/mol×K	938.66	Joback Method
cpg	524.42	J/mol×K	979.06	Joback Method
cpg	531.31	J/mol×K	1019.47	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=U307647&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