6-Bromohexanoic acid, 4-nitrophenyl ester

Inchi: InChI=1S/C12H14BrNO4/c13-9-3-1-2-4-12(15)18-11-7-5-10(6-8-11)14(16)17/h5-8H,1-4,9
InchiKey: IGFDRPHVXMUTLG-UHFFFAOYSA-N
Formula: C12H14BrNO4
SMILES: O=C(CCCCCBr)Oc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 316.15

Physical Properties

Property code	Value	Unit	Source
gf	-31.11	kJ/mol	Joback Method
hf	-295.18	kJ/mol	Joback Method
hfus	39.92	kJ/mol	Joback Method
hvap	77.43	kJ/mol	Joback Method
log10ws	-4.54		Crippen Method
logp	3.455		Crippen Method
mcvol	198.540	ml/mol	McGowan Method
pc	2693.00	kPa	Joback Method
rinpol	2262.00		NIST Webbook
tb	799.91	K	Joback Method
tc	1037.94	K	Joback Method
tf	539.51	K	Joback Method
vc	0.767	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	530.41	J/mol×K	799.91	Joback Method
cpg	542.02	J/mol×K	839.58	Joback Method
cpg	552.68	J/mol×K	879.25	Joback Method
cpg	562.42	J/mol×K	918.93	Joback Method
cpg	571.29	J/mol×K	958.60	Joback Method
cpg	579.34	J/mol×K	998.27	Joback Method
cpg	586.61	J/mol×K	1037.94	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307619&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