6-Bromohexanoic acid, 4-cyanophenyl ester

Inchi: InChI=1S/C13H14BrNO2/c14-9-3-1-2-4-13(16)17-12-7-5-11(10-15)6-8-12/h5-8H,1-4,9H2
InchiKey: DWYXEURUXKFTDN-UHFFFAOYSA-N
Formula: C13H14BrNO2
SMILES: N#Cc1ccc(OC(=O)CCCCCBr)cc1
Mol. weight [g/mol]: 296.16

Physical Properties

Property code	Value	Unit	Source
gf	74.94	kJ/mol	Joback Method
hf	-140.18	kJ/mol	Joback Method
hfus	32.66	kJ/mol	Joback Method
hvap	73.54	kJ/mol	Joback Method
log10ws	-4.24		Crippen Method
logp	3.419		Crippen Method
mcvol	196.590	ml/mol	McGowan Method
pc	2356.49	kPa	Joback Method
rinpol	2130.00		NIST Webbook
tb	773.03	K	Joback Method
tc	999.82	K	Joback Method
tf	472.16	K	Joback Method
vc	0.767	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	505.10	J/mol×K	773.03	Joback Method
cpg	516.49	J/mol×K	810.83	Joback Method
cpg	527.04	J/mol×K	848.63	Joback Method
cpg	536.77	J/mol×K	886.43	Joback Method
cpg	545.74	J/mol×K	924.23	Joback Method
cpg	553.96	J/mol×K	962.02	Joback Method
cpg	561.48	J/mol×K	999.82	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307617&Units=SI

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