5-Bromovaleric acid, 4-cyanophenyl ester

Inchi: InChI=1S/C12H12BrNO2/c13-8-2-1-3-12(15)16-11-6-4-10(9-14)5-7-11/h4-7H,1-3,8H2
InchiKey: YBQWTJJVCQTMTG-UHFFFAOYSA-N
Formula: C12H12BrNO2
SMILES: N#Cc1ccc(OC(=O)CCCCBr)cc1
Mol. weight [g/mol]: 282.13

Physical Properties

Property code	Value	Unit	Source
gf	66.52	kJ/mol	Joback Method
hf	-119.54	kJ/mol	Joback Method
hfus	30.07	kJ/mol	Joback Method
hvap	71.31	kJ/mol	Joback Method
log10ws	-3.83		Crippen Method
logp	3.029		Crippen Method
mcvol	182.500	ml/mol	McGowan Method
pc	2592.49	kPa	Joback Method
rinpol	2013.00		NIST Webbook
tb	750.15	K	Joback Method
tc	980.70	K	Joback Method
tf	460.89	K	Joback Method
vc	0.712	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	453.01	J/mol×K	750.15	Joback Method
cpg	463.88	J/mol×K	788.57	Joback Method
cpg	473.92	J/mol×K	827.00	Joback Method
cpg	483.19	J/mol×K	865.42	Joback Method
cpg	491.70	J/mol×K	903.85	Joback Method
cpg	499.49	J/mol×K	942.27	Joback Method
cpg	506.60	J/mol×K	980.70	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307645&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