4-Bromobutyric acid, 4-cyanophenyl ester

Inchi: InChI=1S/C11H10BrNO2/c12-7-1-2-11(14)15-10-5-3-9(8-13)4-6-10/h3-6H,1-2,7H2
InchiKey: GRWOXAONZBZBSY-UHFFFAOYSA-N
Formula: C11H10BrNO2
SMILES: N#Cc1ccc(OC(=O)CCCBr)cc1
Mol. weight [g/mol]: 268.11

Physical Properties

Property code	Value	Unit	Source
gf	58.10	kJ/mol	Joback Method
hf	-98.90	kJ/mol	Joback Method
hfus	27.48	kJ/mol	Joback Method
hvap	69.09	kJ/mol	Joback Method
log10ws	-3.41		Crippen Method
logp	2.639		Crippen Method
mcvol	168.410	ml/mol	McGowan Method
pc	2865.80	kPa	Joback Method
rinpol	1884.00		NIST Webbook
rinpol	1884.00		NIST Webbook
tb	727.27	K	Joback Method
tc	962.07	K	Joback Method
tf	449.62	K	Joback Method
vc	0.655	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	402.16	J/mol×K	727.27	Joback Method
cpg	412.41	J/mol×K	766.40	Joback Method
cpg	421.87	J/mol×K	805.54	Joback Method
cpg	430.58	J/mol×K	844.67	Joback Method
cpg	438.57	J/mol×K	883.80	Joback Method
cpg	445.87	J/mol×K	922.93	Joback Method
cpg	452.50	J/mol×K	962.07	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=U307610&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