2-Bromopropionic acid, 4-cyanophenyl ester

Inchi: InChI=1S/C10H8BrNO2/c1-7(11)10(13)14-9-4-2-8(6-12)3-5-9/h2-5,7H,1H3
InchiKey: FAAGNDLVLVABEZ-UHFFFAOYSA-N
Formula: C10H8BrNO2
SMILES: CC(Br)C(=O)Oc1ccc(C#N)cc1
Mol. weight [g/mol]: 254.08

Physical Properties

Property code	Value	Unit	Source
gf	47.24	kJ/mol	Joback Method
hf	-83.54	kJ/mol	Joback Method
hfus	21.36	kJ/mol	Joback Method
hvap	66.47	kJ/mol	Joback Method
log10ws	-3.10		Crippen Method
logp	2.247		Crippen Method
mcvol	154.320	ml/mol	McGowan Method
pc	3213.68	kPa	Joback Method
rinpol	1643.00		NIST Webbook
rinpol	1643.00		NIST Webbook
tb	703.95	K	Joback Method
tc	948.30	K	Joback Method
tf	423.35	K	Joback Method
vc	0.594	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	353.23	J/mol×K	703.95	Joback Method
cpg	362.98	J/mol×K	744.67	Joback Method
cpg	371.94	J/mol×K	785.40	Joback Method
cpg	380.13	J/mol×K	826.12	Joback Method
cpg	387.60	J/mol×K	866.85	Joback Method
cpg	394.37	J/mol×K	907.57	Joback Method
cpg	400.46	J/mol×K	948.30	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308025&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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