4-Bromobutyric acid, pentafluorophenyl ester

Inchi: InChI=1S/C10H6BrF5O2/c11-3-1-2-4(17)18-10-8(15)6(13)5(12)7(14)9(10)16/h1-3H2
InchiKey: WBMIQBCBWZHXQZ-UHFFFAOYSA-N
Formula: C10H6BrF5O2
SMILES: O=C(CCCBr)Oc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 333.05

Physical Properties

Property code	Value	Unit	Source
gf	-1096.07	kJ/mol	Joback Method
hf	-1269.57	kJ/mol	Joback Method
hfus	37.22	kJ/mol	Joback Method
hvap	54.95	kJ/mol	Joback Method
log10ws	-4.71		Crippen Method
logp	3.463		Crippen Method
mcvol	161.790	ml/mol	McGowan Method
pc	2421.88	kPa	Joback Method
rinpol	1473.00		NIST Webbook
tb	618.58	K	Joback Method
tc	803.37	K	Joback Method
tf	426.39	K	Joback Method
vc	0.663	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	373.65	J/mol×K	618.58	Joback Method
cpg	382.51	J/mol×K	649.38	Joback Method
cpg	390.94	J/mol×K	680.18	Joback Method
cpg	398.95	J/mol×K	710.98	Joback Method
cpg	406.53	J/mol×K	741.78	Joback Method
cpg	413.68	J/mol×K	772.58	Joback Method
cpg	420.41	J/mol×K	803.37	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=U354685&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