

5-Bromovaleric acid, 4-chlorophenyl ester

Inchi:	InChI=1S/C11H12BrClO2/c12-8-2-1-3-11(14)15-10-6-4-9(13)5-7-10/h4-7H,1-3,8H2
InchiKey:	IMWJAQXFZRMLJX-UHFFFAOYSA-N
Formula:	C11H12BrClO2
SMILES:	O=C(CCCCBBr)Oc1ccc(Cl)cc1
Mol. weight [g/mol]:	291.57

Physical Properties

Property code	Value	Unit	Source
gf	-87.01	kJ/mol	Joback Method
hf	-279.52	kJ/mol	Joback Method
hfus	30.17	kJ/mol	Joback Method
hvap	62.99	kJ/mol	Joback Method
log10ws	-4.16		Crippen Method
logp	3.811		Crippen Method
mvol	179.270	ml/mol	McGowan Method
pc	2829.33	kPa	Joback Method
rpol	1879.00		NIST Webbook
tb	662.62	K	Joback Method
tc	888.74	K	Joback Method
tf	414.55	K	Joback Method
vc	0.678	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	408.92	J/molxK	662.62	Joback Method
cpg	461.31	J/molxK	851.06	Joback Method
cpg	452.36	J/molxK	813.37	Joback Method
cpg	442.68	J/molxK	775.68	Joback Method
cpg	432.23	J/molxK	737.99	Joback Method
cpg	420.99	J/molxK	700.31	Joback Method
cpg	469.55	J/molxK	888.74	Joback Method
dvisc	0.0001758	Paxs	662.62	Joback Method
dvisc	0.0002183	Paxs	621.27	Joback Method

dvisc	0.0002795	Paxs	579.93	Joback Method
dvisc	0.0003716	Paxs	538.59	Joback Method
dvisc	0.0005181	Paxs	497.24	Joback Method
dvisc	0.0007672	Paxs	455.89	Joback Method
dvisc	0.0012288	Paxs	414.55	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U307642&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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

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