

5-Bromovaleric acid, hexyl ester

Inchi:	InChI=1S/C11H21BrO2/c1-2-3-4-7-10-14-11(13)8-5-6-9-12/h2-10H2,1H3
InchiKey:	BXBXNTGHTDMQIS-UHFFFAOYSA-N
Formula:	C11H21BrO2
SMILES:	CCCCCOC(=O)CCCCBr
Mol. weight [g/mol]:	265.19
CAS:	13931-42-5

Physical Properties

Property code	Value	Unit	Source
gf	-177.86	kJ/mol	Joback Method
hf	-488.84	kJ/mol	Joback Method
hfus	32.32	kJ/mol	Joback Method
hvap	55.67	kJ/mol	Joback Method
log10ws	-3.72		Crippen Method
logp	3.675		Crippen Method
mcvol	190.790	ml/mol	McGowan Method
pc	2145.33	kPa	Joback Method
rinpol	1635.70		NIST Webbook
rinpol	1635.70		NIST Webbook
tb	593.53	K	Joback Method
tc	777.06	K	Joback Method
tf	345.69	K	Joback Method
vc	0.738	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	461.92	J/molxK	593.53	Joback Method
cpg	476.21	J/molxK	624.12	Joback Method
cpg	489.85	J/molxK	654.71	Joback Method
cpg	502.85	J/molxK	685.30	Joback Method
cpg	515.24	J/molxK	715.88	Joback Method
cpg	527.02	J/molxK	746.47	Joback Method
cpg	538.21	J/molxK	777.06	Joback Method

dvisc	0.0021937	Paxs	345.69	Joback Method
dvisc	0.0011833	Paxs	387.00	Joback Method
dvisc	0.0007190	Paxs	428.30	Joback Method
dvisc	0.0004769	Paxs	469.61	Joback Method
dvisc	0.0003380	Paxs	510.92	Joback Method
dvisc	0.0002522	Paxs	552.22	Joback Method
dvisc	0.0001961	Paxs	593.53	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13931425&Units=SI
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

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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