

5-Bromovaleric acid, pentyl ester

Inchi:	InChI=1S/C10H19BrO2/c1-2-3-6-9-13-10(12)7-4-5-8-11/h2-9H2,1H3
InchiKey:	FMNQYYCJDDZAHH-UHFFFAOYSA-N
Formula:	C10H19BrO2
SMILES:	CCCCCOC(=O)CCCCBr
Mol. weight [g/mol]:	251.16
CAS:	13931-41-4

Physical Properties

Property code	Value	Unit	Source
gf	-186.28	kJ/mol	Joback Method
hf	-468.20	kJ/mol	Joback Method
hfus	29.73	kJ/mol	Joback Method
hvap	53.45	kJ/mol	Joback Method
log10ws	-3.30		Crippen Method
logp	3.285		Crippen Method
mvol	176.700	ml/mol	McGowan Method
pc	2349.64	kPa	Joback Method
rinpol	1537.50		NIST Webbook
rinpol	1537.50		NIST Webbook
tb	570.65	K	Joback Method
tc	756.07	K	Joback Method
tf	334.42	K	Joback Method
vc	0.681	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	412.99	J/molxK	570.65	Joback Method
cpg	426.59	J/molxK	601.55	Joback Method
cpg	439.57	J/molxK	632.46	Joback Method
cpg	451.95	J/molxK	663.36	Joback Method
cpg	463.74	J/molxK	694.27	Joback Method
cpg	474.96	J/molxK	725.17	Joback Method
cpg	485.63	J/molxK	756.07	Joback Method

dvisc	0.0023247	Paxs	334.42	Joback Method
dvisc	0.0012758	Paxs	373.79	Joback Method
dvisc	0.0007850	Paxs	413.16	Joback Method
dvisc	0.0005256	Paxs	452.53	Joback Method
dvisc	0.0003752	Paxs	491.91	Joback Method
dvisc	0.0002816	Paxs	531.28	Joback Method
dvisc	0.0002199	Paxs	570.65	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13931414&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
mvol:	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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