

2- Bromopropionic acid, pentyl ester

Other names:	Propanoic acid, 2-bromo, pentyl ester Pentyl 2-bromopropanoate
Inchi:	InChI=1S/C8H15BrO2/c1-3-4-5-6-11-8(10)7(2)9/h7H,3-6H2,1-2H3
InchiKey:	IJSDPKDUSUXUFY-UHFFFAOYSA-N
Formula:	C8H15BrO2
SMILES:	CCCCCOC(=O)C(C)Br
Mol. weight [g/mol]:	223.11
CAS:	86711-73-1

Physical Properties

Property code	Value	Unit	Source
gf	-205.56	kJ/mol	Joback Method
hf	-432.20	kJ/mol	Joback Method
hfus	21.02	kJ/mol	Joback Method
hvap	48.61	kJ/mol	Joback Method
log10ws	-2.58		Crippen Method
logp	2.503		Crippen Method
mcvol	148.520	ml/mol	McGowan Method
pc	2881.21	kPa	Joback Method
rinpol	1198.00		NIST Webbook
rinpol	1213.60		NIST Webbook
rinpol	1213.60		NIST Webbook
rinpol	1194.00		NIST Webbook
rinpol	1198.00		NIST Webbook
ripol	1584.00		NIST Webbook
ripol	1584.00		NIST Webbook
tb	524.45	K	Joback Method
tc	718.18	K	Joback Method
tf	296.88	K	Joback Method
vc	0.564	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	320.63	J/mol×K	524.45	Joback Method
cpg	376.32	J/mol×K	685.89	Joback Method
cpg	366.25	J/mol×K	653.60	Joback Method
cpg	355.66	J/mol×K	621.31	Joback Method
cpg	344.53	J/mol×K	589.03	Joback Method
cpg	332.86	J/mol×K	556.74	Joback Method
cpg	385.87	J/mol×K	718.18	Joback Method
dvisc	0.0002562	Pa×s	524.45	Joback Method
dvisc	0.0003325	Pa×s	486.52	Joback Method
dvisc	0.0004510	Pa×s	448.59	Joback Method
dvisc	0.0006473	Pa×s	410.67	Joback Method
dvisc	0.0009998	Pa×s	372.74	Joback Method
dvisc	0.0017041	Pa×s	334.81	Joback Method
dvisc	0.0033286	Pa×s	296.88	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=C86711731&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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature

tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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