

Propanoic acid, 3-bromo, butyl ester

Other names:	Butyl 3-bromopropanoate
Inchi:	InChI=1S/C7H13BrO2/c1-2-3-6-10-7(9)4-5-8/h2-6H2,1H3
InchiKey:	QDEAPWRQCUZSEZ-UHFFFAOYSA-N
Formula:	C7H13BrO2
SMILES:	CCCCOC(=O)CCBr
Mol. weight [g/mol]:	209.08

Physical Properties

Property code	Value	Unit	Source
gf	-211.54	kJ/mol	Joback Method
hf	-406.28	kJ/mol	Joback Method
hfus	21.96	kJ/mol	Joback Method
hvap	46.77	kJ/mol	Joback Method
log10ws	-2.05		Crippen Method
logp	2.115		Crippen Method
mcvol	134.430	ml/mol	McGowan Method
pc	3173.97	kPa	Joback Method
ripol	1175.00		NIST Webbook
ripol	1646.00		NIST Webbook
ripol	1646.00		NIST Webbook
tb	502.01	K	Joback Method
tc	694.06	K	Joback Method
tf	300.61	K	Joback Method
vc	0.513	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	276.81	J/molxK	502.01	Joback Method
cpg	326.65	J/molxK	662.05	Joback Method
cpg	317.59	J/molxK	630.04	Joback Method
cpg	308.09	J/molxK	598.04	Joback Method
cpg	298.13	J/molxK	566.03	Joback Method
cpg	287.70	J/molxK	534.02	Joback Method

cpg	335.26	J/molxK	694.06	Joback Method
dvisc	0.0002990	Paxs	502.01	Joback Method
dvisc	0.0003769	Paxs	468.44	Joback Method
dvisc	0.0004925	Paxs	434.88	Joback Method
dvisc	0.0006729	Paxs	401.31	Joback Method
dvisc	0.0009732	Paxs	367.74	Joback Method
dvisc	0.0015160	Paxs	334.18	Joback Method
dvisc	0.0026071	Paxs	300.61	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R30090&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

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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