Propyl 3-bromopropanoate

Other names: Propanoic acid, 3-bromo, propyl ester
Inchi: InChI=1S/C6H11BrO2/c1-2-5-9-6(8)3-4-7/h2-5H2,1H3
InchiKey: DXFHVUUGWSXHQY-UHFFFAOYSA-N
Formula: C6H11BrO2
SMILES: CCCOC(=O)CCBr
Mol. weight [g/mol]: 195.05

Physical Properties

Property code	Value	Unit	Source
gf	-219.96	kJ/mol	Joback Method
hf	-385.64	kJ/mol	Joback Method
hfus	19.37	kJ/mol	Joback Method
hvap	44.54	kJ/mol	Joback Method
log10ws	-1.63		Crippen Method
logp	1.725		Crippen Method
mcvol	120.340	ml/mol	McGowan Method
pc	3547.31	kPa	Joback Method
rinpol	1077.00		NIST Webbook
tb	479.13	K	Joback Method
tc	673.53	K	Joback Method
tf	289.34	K	Joback Method
vc	0.458	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	235.29	J/mol×K	479.13	Joback Method
cpg	280.00	J/mol×K	641.13	Joback Method
cpg	271.87	J/mol×K	608.73	Joback Method
cpg	263.33	J/mol×K	576.33	Joback Method
cpg	254.40	J/mol×K	543.93	Joback Method
cpg	245.05	J/mol×K	511.53	Joback Method
cpg	287.75	J/mol×K	673.53	Joback Method
dvisc	0.0003263	Pa×s	479.13	Joback Method

dvisc	0.0004089	Pa×s	447.50	Joback Method
dvisc	0.0005301	Pa×s	415.87	Joback Method
dvisc	0.0007175	Pa×s	384.24	Joback Method
dvisc	0.0010251	Pa×s	352.60	Joback Method
dvisc	0.0015715	Pa×s	320.97	Joback Method
dvisc	0.0026449	Pa×s	289.34	Joback Method

Sources

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=R30371&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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