Propyl 2-bromopropanoate

Other names: Propanoic acid, 2-bromo, propyl ester
Inchi: InChI=1S/C6H11BrO2/c1-3-4-9-6(8)5(2)7/h5H,3-4H2,1-2H3
InchiKey: GDPGCHFFZZXKTQ-UHFFFAOYSA-N
Formula: C6H11BrO2
SMILES: CCCOC(=O)C(C)Br
Mol. weight [g/mol]: 195.05

Physical Properties

Property code	Value	Unit	Source
gf	-222.40	kJ/mol	Joback Method
hf	-390.92	kJ/mol	Joback Method
hfus	15.85	kJ/mol	Joback Method
hvap	44.15	kJ/mol	Joback Method
log10ws	-1.74		Crippen Method
logp	1.723		Crippen Method
mcvol	120.340	ml/mol	McGowan Method
pc	3581.35	kPa	Joback Method
rinpol	1005.00		NIST Webbook
ripol	1405.00		NIST Webbook
tb	478.69	K	Joback Method
tc	677.47	K	Joback Method
tf	274.34	K	Joback Method
vc	0.452	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	235.52	J/mol×K	478.69	Joback Method
cpg	281.46	J/mol×K	644.34	Joback Method
cpg	273.13	J/mol×K	611.21	Joback Method
cpg	264.38	J/mol×K	578.08	Joback Method
cpg	255.20	J/mol×K	544.95	Joback Method
cpg	245.58	J/mol×K	511.82	Joback Method
cpg	289.37	J/mol×K	677.47	Joback Method

dvisc	0.0003098	Pa×s	478.69	Joback Method
dvisc	0.0003980	Pa×s	444.63	Joback Method
dvisc	0.0005331	Pa×s	410.57	Joback Method
dvisc	0.0007528	Pa×s	376.51	Joback Method
dvisc	0.0011385	Pa×s	342.46	Joback Method
dvisc	0.0018866	Pa×s	308.40	Joback Method
dvisc	0.0035442	Pa×s	274.34	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R23269&Units=SI
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

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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