

Isopropyl 3-bromopropanoate

Other names:	Propanoic acid, 3-bromo, isopropyl ester
Inchi:	InChI=1S/C6H11BrO2/c1-5(2)9-6(8)3-4-7/h5H,3-4H2,1-2H3
InchiKey:	KQNJUTDIDREYGN-UHFFFAOYSA-N
Formula:	C6H11BrO2
SMILES:	CC(C)OC(=O)CCBr
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
ripol	1466.00		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/molxK	478.69	Joback Method
cpg	245.58	J/molxK	511.82	Joback Method
cpg	255.20	J/molxK	544.95	Joback Method
cpg	264.38	J/molxK	578.08	Joback Method
cpg	273.13	J/molxK	611.21	Joback Method
cpg	281.46	J/molxK	644.34	Joback Method
cpg	289.37	J/molxK	677.47	Joback Method
dvisc	0.0035442	Paxs	274.34	Joback Method

dvisc	0.0018866	Paxs	308.40	Joback Method
dvisc	0.0011385	Paxs	342.46	Joback Method
dvisc	0.0007528	Paxs	376.51	Joback Method
dvisc	0.0005331	Paxs	410.57	Joback Method
dvisc	0.0003980	Paxs	444.63	Joback Method
dvisc	0.0003098	Paxs	478.69	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R30161&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
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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