Pentyl 3-bromopropanoate

Other names: Propanoic acid, 3-bromo, pentyl ester
Inchi: InChI=1S/C8H15BrO2/c1-2-3-4-7-11-8(10)5-6-9/h2-7H2,1H3
InchiKey: RXZKJMDTKJNLJR-UHFFFAOYSA-N
Formula: C8H15BrO2
SMILES: CCCCCOC(=O)CCBr
Mol. weight [g/mol]: 223.11

Physical Properties

Property code	Value	Unit	Source
gf	-203.12	kJ/mol	Joback Method
hf	-426.92	kJ/mol	Joback Method
hfus	24.55	kJ/mol	Joback Method
hvap	48.99	kJ/mol	Joback Method
log10ws	-2.47		Crippen Method
logp	2.505		Crippen Method
mcvol	148.520	ml/mol	McGowan Method
pc	2856.62	kPa	Joback Method
rinpol	1273.00		NIST Webbook
rinpol	1273.00		NIST Webbook
ripol	1740.00		NIST Webbook
tb	524.89	K	Joback Method
tc	714.63	K	Joback Method
tf	311.88	K	Joback Method
vc	0.570	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	320.33	J/mol×K	524.89	Joback Method
cpg	374.73	J/mol×K	683.00	Joback Method
cpg	364.86	J/mol×K	651.38	Joback Method
cpg	354.49	J/mol×K	619.76	Joback Method
cpg	343.62	J/mol×K	588.14	Joback Method
cpg	332.24	J/mol×K	556.51	Joback Method

cpg	384.11	J/mol×K	714.63	Joback Method
dvisc	0.0002718	Pa×s	524.89	Joback Method
dvisc	0.0003445	Pa×s	489.39	Joback Method
dvisc	0.0004533	Pa×s	453.89	Joback Method
dvisc	0.0006249	Pa×s	418.38	Joback Method
dvisc	0.0009142	Pa×s	382.88	Joback Method
dvisc	0.0014455	Pa×s	347.38	Joback Method
dvisc	0.0025371	Pa×s	311.88	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=R30189&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume