Propyl bromoacetate

Other names: Propyl bromoacetate
Inchi: InChI=1S/C5H9BrO2/c1-2-3-8-5(7)4-6/h2-4H2,1H3
InchiKey: ISYUCUGTDNJIHV-UHFFFAOYSA-N
Formula: C5H9BrO2
SMILES: CCCOC(=O)CBr
Mol. weight [g/mol]: 181.03

Physical Properties

Property code	Value	Unit	Source
hf	-451.44	kJ/mol	Cheméo Relay (1.0)
hfus	16.78	kJ/mol	Joback Method
hvap	46.22	kJ/mol	Cheméo Relay (1.0)
ie	10.11	eV	Cheméo Relay (1.0)
log10ws	-1.57		Cheméo Relay (1.0)
logp	1.334		Crippen Method
mcvol	106.250	ml/mol	McGowan Method
pc	3990.60	kPa	Joback Method
rinpol	969.50		NIST Webbook
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tb	449.20	K	NIST Webbook
tc	627.07	K	Cheméo Relay (1.0)
tf	240.49	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	195.91	J/mol×K	456.25	Joback Method
cpg	204.39	J/mol×K	489.03	Joback Method
cpg	212.52	J/mol×K	521.82	Joback Method
cpg	220.31	J/mol×K	554.60	Joback Method
cpg	227.76	J/mol×K	587.39	Joback Method
cpg	234.86	J/mol×K	620.17	Joback Method
cpg	241.64	J/mol×K	652.96	Joback Method
dvisc	0.0026445	Pa×s	278.07	Joback Method

dvisc	0.0016076	Pa×s	307.77	Joback Method
dvisc	0.0010668	Pa×s	337.46	Joback Method
dvisc	0.0007565	Pa×s	367.16	Joback Method
dvisc	0.0005647	Pa×s	396.86	Joback Method
dvisc	0.0004391	Pa×s	426.55	Joback Method
dvisc	0.0003528	Pa×s	456.25	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C35223804&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
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