Ethyl 2-bromovalerate

Other names:	Ethyl «alpha»-bromovalerate
	Pentanoic acid, 2-bromo-, ethyl ester
	Ethanol, 2-bromopentanoate
Inchi:	InChI=1S/C7H13BrO2/c1-3-5-6(8)7(9)10-4-2/h6H,3-5H2,1-2H3
InchiKey:	ORSIRXYHFPHWTN-UHFFFAOYSA-N
Formula:	C7H13BrO2
SMILES:	CCCC(Br)C(=O)OCC
Mol. weight [g/mol]:	209.08
CAS:	615-83-8

Physical Properties

Property code	Value	Unit	Source
gf	-213.98	kJ/mol	Joback Method
hf	-411.56	kJ/mol	Joback Method
hfus	18.43	kJ/mol	Joback Method
hvap	46.38	kJ/mol	Joback Method
log10ws	-2.16		Crippen Method
logp	2.113		Crippen Method
mcvol	134.430	ml/mol	McGowan Method
pc	3202.78	kPa	Joback Method
rinpol	1163.00		NIST Webbook
rinpol	1085.00		NIST Webbook
rinpol	1085.00		NIST Webbook
tb	464.20	K	NIST Webbook
tc	697.81	K	Joback Method
tf	285.61	K	Joback Method
vc	0.507	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	277.07	J/mol×K	501.57	Joback Method
cpg	288.28	J/mol×K	534.28	Joback Method
cpg	298.99	J/mol×K	566.98	Joback Method

cpg	309.20	J/mol×K	599.69	Joback Method
cpg	318.93	J/mol×K	632.40	Joback Method
cpg	328.18	J/mol×K	665.11	Joback Method
cpg	336.97	J/mol×K	697.81	Joback Method
dvisc	0.0034561	Pa×s	285.61	Joback Method
dvisc	0.0018031	Pa×s	321.60	Joback Method
dvisc	0.0010723	Pa×s	357.60	Joback Method
dvisc	0.0007013	Pa×s	393.59	Joback Method
dvisc	0.0004925	Pa×s	429.58	Joback Method
dvisc	0.0003653	Pa×s	465.58	Joback Method
dvisc	0.0002828	Pa×s	501.57	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C615838&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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