ETHYL 4-BROMOBUTYRATE

Other names:	BrCH2CH2CH2C(O)OC2H5
	Ethyl «gamma»-bromobutyrate
	Butanoic acid, 4-bromo-, ethyl ester
	4-Bromobutanoic acid, ethyl ester
Inchi:	InChI=1S/C6H11BrO2/c1-2-9-6(8)4-3-5-7/h2-5H2,1H3
InchiKey:	XBPOBCXHALHJFP-UHFFFAOYSA-N
Formula:	C6H11BrO2
SMILES:	CCOC(=O)CCCBr
Mol. weight [g/mol]:	195.06

Physical Properties

Property code	Value	Unit	Source
af	0.5582		Cheméo Relay (1.0)
gf	-219.96	kJ/mol	Joback Method
hf	-466.03	kJ/mol	Cheméo Relay (1.0)
hfus	19.37	kJ/mol	Joback Method
hvap	55.09	kJ/mol	Cheméo Relay (1.0)
ie	9.86	eV	Cheméo Relay (1.0)
log10ws	-1.62		Cheméo Relay (1.0)
logp	1.725		Crippen Method
mcvol	120.340	ml/mol	McGowan Method
pc	3547.31	kPa	Joback Method
tb	468.58	K	Cheméo Relay (1.0)
tc	645.26	K	Cheméo Relay (1.0)
tf	226.05	K	Cheméo Relay (1.0)
vc	0.439	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	235.29	J/mol×K	479.13	Joback Method
cpg	245.05	J/mol×K	511.53	Joback Method
cpg	254.40	J/mol×K	543.93	Joback Method
cpg	263.33	J/mol×K	576.33	Joback Method

cpg	271.87	J/mol×K	608.73	Joback Method
cpg	280.00	J/mol×K	641.13	Joback Method
cpg	287.75	J/mol×K	673.53	Joback Method
dvisc	0.0026449	Pa×s	289.34	Joback Method
dvisc	0.0015715	Pa×s	320.97	Joback Method
dvisc	0.0010251	Pa×s	352.60	Joback Method
dvisc	0.0007175	Pa×s	384.24	Joback Method
dvisc	0.0005301	Pa×s	415.87	Joback Method
dvisc	0.0004089	Pa×s	447.50	Joback Method
dvisc	0.0003263	Pa×s	479.13	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	355.20	K	1.30	NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2969815&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

Legend

af: Acentric Factor
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

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume