

Ethyl 4-bromobutyrate

Other names:	BrCH ₂ CH ₂ CH ₂ C(O)OC ₂ H ₅ 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:	C ₆ H ₁₁ BrO ₂
SMILES:	CCOC(=O)CCCB
Mol. weight [g/mol]:	195.05
CAS:	2969-81-5

Physical Properties

Property code	Value	Unit	Source
gf	-219.96	kJ/mol	Joback Method
hf	-385.64	kJ/mol	Joback Method
hfus	19.37	kJ/mol	Joback Method
hvap	44.54	kJ/mol	Joback Method
log10ws	-1.63		Crippen Method
logp	1.725		Crippen Method
mcvol	120.340	ml/mol	McGowan Method
pc	3547.31	kPa	Joback Method
tb	479.13	K	Joback Method
tc	673.53	K	Joback Method
tf	289.34	K	Joback Method
vc	0.458	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	235.29	J/mol×K	479.13	Joback Method
cpg	280.00	J/mol×K	641.13	Joback Method
cpg	271.87	J/mol×K	608.73	Joback Method
cpg	263.33	J/mol×K	576.33	Joback Method
cpg	254.40	J/mol×K	543.93	Joback Method

cpg	245.05	J/molxK	511.53	Joback Method
cpg	287.75	J/molxK	673.53	Joback Method
dvisc	0.0003263	Paxs	479.13	Joback Method
dvisc	0.0004089	Paxs	447.50	Joback Method
dvisc	0.0005301	Paxs	415.87	Joback Method
dvisc	0.0007175	Paxs	384.24	Joback Method
dvisc	0.0010251	Paxs	352.60	Joback Method
dvisc	0.0015715	Paxs	320.97	Joback Method
dvisc	0.0026449	Paxs	289.34	Joback Method

Pressure Dependent Properties

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

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2969815&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
mvol:	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

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