Ethyl «alpha»-bromocyclobutanecarboxylate

Other names:	Cyclobutanecarboxylic acid, 1-bromo-, ethyl ester
	Ethyl 1-bromocyclobutanecarboxylate
Inchi:	InChI=1S/C7H11BrO2/c1-2-10-6(9)7(8)4-3-5-7/h2-5H2,1H3
InchiKey:	UTVNSHXHFRIXMM-UHFFFAOYSA-N
Formula:	C7H11BrO2
SMILES:	CCOC(=O)C1(Br)CCC1
Mol. weight [g/mol]:	207.06
CAS:	35120-18-4

Physical Properties

Property code	Value	Unit	Source
gf	-168.38	kJ/mol	Joback Method
hf	-324.40	kJ/mol	Joback Method
hfus	11.69	kJ/mol	Joback Method
hvap	45.70	kJ/mol	Joback Method
log10ws	-2.05		Crippen Method
logp	1.867		Crippen Method
mcvol	123.570	ml/mol	McGowan Method
pc	4031.24	kPa	Joback Method
tb	513.26	K	Joback Method
tc	737.17	K	Joback Method
tf	338.93	K	Joback Method
vc	0.461	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	261.27	J/mol×K	513.26	Joback Method
cpg	273.50	J/mol×K	550.58	Joback Method
cpg	284.81	J/mol×K	587.90	Joback Method
cpg	295.34	J/mol×K	625.21	Joback Method
cpg	305.21	J/mol×K	662.53	Joback Method
cpg	314.55	J/mol×K	699.85	Joback Method
cpg	323.48	J/mol×K	737.17	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	359.70	K	1.60	NIST Webbook

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=C35120184&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
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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume