

Acetic acid, bromo-, ethyl ester

Other names:	Antol Bromoacetic acid ethyl ester Ethoxycarbonylmethyl bromide Ethyl «alpha»-bromoacetate Ethyl bromacetate Ethyl bromoacetate Ethyl monobromoacetate UN 1603 Acetic acid, 2-bromo-, ethyl ester Ethyl 2-bromoacetate NSC 8832
Inchi:	InChI=1S/C4H7BrO2/c1-2-7-4(6)3-5/h2-3H2,1H3
InchiKey:	PQJJJMRNHATNKG-UHFFFAOYSA-N
Formula:	C4H7BrO2
SMILES:	CCOC(=O)CBr
Mol. weight [g/mol]:	167.00
CAS:	105-36-2

Physical Properties

Property code	Value	Unit	Source
gf	-236.80	kJ/mol	Joback Method
hf	-344.36	kJ/mol	Joback Method
hfus	14.19	kJ/mol	Joback Method
hvap	40.09	kJ/mol	Joback Method
log10ws	-0.79		Crippen Method
logp	0.944		Crippen Method
mcvol	92.160	ml/mol	McGowan Method
pc	4522.49	kPa	Joback Method
tb	433.37	K	Joback Method
tc	632.29	K	Joback Method
tf	266.80	K	Joback Method
vc	0.345	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	158.76	J/molxK	433.37	Joback Method
cpg	165.82	J/molxK	466.52	Joback Method
cpg	172.60	J/molxK	499.68	Joback Method
cpg	179.11	J/molxK	532.83	Joback Method
cpg	185.34	J/molxK	565.98	Joback Method
cpg	191.30	J/molxK	599.13	Joback Method
cpg	196.99	J/molxK	632.29	Joback Method
dvisc	0.0026007	Paxs	266.80	Joback Method
dvisc	0.0016199	Paxs	294.56	Joback Method
dvisc	0.0010947	Paxs	322.32	Joback Method
dvisc	0.0007873	Paxs	350.09	Joback Method
dvisc	0.0005942	Paxs	377.85	Joback Method
dvisc	0.0004662	Paxs	405.61	Joback Method
dvisc	0.0003772	Paxs	433.37	Joback Method

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=C105362&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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