

5-Bromovaleric acid, cyclobutyl ester

Inchi:	InChI=1S/C9H15BrO2/c10-7-2-1-6-9(11)12-8-4-3-5-8/h8H,1-7H2
InchiKey:	GWVUWXKSZDXMHL-UHFFFAOYSA-N
Formula:	C9H15BrO2
SMILES:	O=C(CCCCBBr)OC1CCC1
Mol. weight [g/mol]:	235.12

Physical Properties

Property code	Value	Unit	Source
gf	-146.05	kJ/mol	Joback Method
hf	-380.92	kJ/mol	Joback Method
hfus	23.17	kJ/mol	Joback Method
hvap	51.30	kJ/mol	Joback Method
log10ws	-2.89		Crippen Method
logp	2.647		Crippen Method
mcvol	151.750	ml/mol	McGowan Method
pc	3045.68	kPa	Joback Method
rinqol	1438.00		NIST Webbook
tb	558.78	K	Joback Method
tc	766.68	K	Joback Method
tf	337.57	K	Joback Method
vc	0.575	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	351.76	J/molxK	558.78	Joback Method
cpg	415.37	J/molxK	732.03	Joback Method
cpg	404.15	J/molxK	697.38	Joback Method
cpg	392.21	J/molxK	662.73	Joback Method
cpg	379.52	J/molxK	628.08	Joback Method
cpg	366.05	J/molxK	593.43	Joback Method
cpg	425.92	J/molxK	766.68	Joback Method
dvisc	0.0004285	Paxs	558.78	Joback Method
dvisc	0.0005185	Paxs	521.91	Joback Method

dvisc	0.0006459	Paxs	485.04	Joback Method
dvisc	0.0008342	Paxs	448.17	Joback Method
dvisc	0.0011279	Paxs	411.31	Joback Method
dvisc	0.0016185	Paxs	374.44	Joback Method
dvisc	0.0025130	Paxs	337.57	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299979&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
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

Latest version available from:

<https://www.chemeo.com/cid/31-919-7/5-Bromovaleric-acid-cyclobutyl-ester.pdf>

Generated by Cheméo on 2024-05-05 02:43:27.974703289 +0000 UTC m=+17166256.895280611.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.