

Hexanoic acid, 2-bromo-, ethyl ester

Other names:	«alpha»-Bromocaproic acid, ethyl ester Ethyl «alpha»-bromocaproate Ethyl 2-bromocaproate Ethyl 2-bromohexanoate 2-Bromohexanoic acid ethyl ester
Inchi:	InChI=1S/C8H15BrO2/c1-3-5-6-7(9)8(10)11-4-2/h7H,3-6H2,1-2H3
InchiKey:	KOUAQOCYMAENKN-UHFFFAOYSA-N
Formula:	C8H15BrO2
SMILES:	CCCCC(Br)C(=O)OCC
Mol. weight [g/mol]:	223.11
CAS:	615-96-3

Physical Properties

Property code	Value	Unit	Source
gf	-205.56	kJ/mol	Joback Method
hf	-432.20	kJ/mol	Joback Method
hfus	21.02	kJ/mol	Joback Method
hvap	48.61	kJ/mol	Joback Method
log10ws	-2.58		Crippen Method
logp	2.503		Crippen Method
mcvol	148.520	ml/mol	McGowan Method
pc	2881.21	kPa	Joback Method
tb	487.20	K	NIST Webbook
tc	718.18	K	Joback Method
tf	296.88	K	Joback Method
vc	0.564	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	320.63	J/molxK	524.45	Joback Method
cpg	376.32	J/molxK	685.89	Joback Method
cpg	366.25	J/molxK	653.60	Joback Method
cpg	355.66	J/molxK	621.31	Joback Method

cpg	344.53	J/molxK	589.03	Joback Method
cpg	332.86	J/molxK	556.74	Joback Method
cpg	385.87	J/molxK	718.18	Joback Method
dvisc	0.0002562	Paxs	524.45	Joback Method
dvisc	0.0003325	Paxs	486.52	Joback Method
dvisc	0.0004510	Paxs	448.59	Joback Method
dvisc	0.0006473	Paxs	410.67	Joback Method
dvisc	0.0009998	Paxs	372.74	Joback Method
dvisc	0.0017041	Paxs	334.81	Joback Method
dvisc	0.0033286	Paxs	296.88	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C615963&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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