

Hexanoic acid, 2-bromoethyl ester

Inchi:	InChI=1S/C8H15BrO2/c1-2-3-4-5-8(10)11-7-6-9/h2-7H2,1H3
InchiKey:	AHELICBDMBDYSN-UHFFFAOYSA-N
Formula:	C8H15BrO2
SMILES:	CCCCCC(=O)OCCBr
Mol. weight [g/mol]:	223.11
CAS:	6282-52-6

Physical Properties

Property code	Value	Unit	Source
gf	-203.12	kJ/mol	Joback Method
hf	-426.92	kJ/mol	Joback Method
hfus	24.55	kJ/mol	Joback Method
hvap	48.99	kJ/mol	Joback Method
log10ws	-2.47		Crippen Method
logp	2.505		Crippen Method
mcvol	148.520	ml/mol	McGowan Method
pc	2856.62	kPa	Joback Method
rinpol	1282.00		NIST Webbook
rinpol	1261.00		NIST Webbook
rinpol	1261.00		NIST Webbook
tb	524.89	K	Joback Method
tc	714.63	K	Joback Method
tf	311.88	K	Joback Method
vc	0.570	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	320.33	J/molxK	524.89	Joback Method
cpg	332.24	J/molxK	556.51	Joback Method
cpg	343.62	J/molxK	588.14	Joback Method
cpg	354.49	J/molxK	619.76	Joback Method
cpg	364.86	J/molxK	651.38	Joback Method
cpg	374.73	J/molxK	683.00	Joback Method

cpg	384.11	J/mol×K	714.63	Joback Method
dvisc	0.0025371	Paxs	311.88	Joback Method
dvisc	0.0014455	Paxs	347.38	Joback Method
dvisc	0.0009142	Paxs	382.88	Joback Method
dvisc	0.0006249	Paxs	418.38	Joback Method
dvisc	0.0004533	Paxs	453.89	Joback Method
dvisc	0.0003445	Paxs	489.39	Joback Method
dvisc	0.0002718	Paxs	524.89	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6282526&Units=SI

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

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