Bromoacetic acid, hexyl ester

Other names: Hexyl bromoacetate
Inchi: InChI=1S/C8H15BrO2/c1-2-3-4-5-6-11-8(10)7-9/h2-7H2,1H3
InchiKey: NNPJKFMGVZNJHG-UHFFFAOYSA-N
Formula: C8H15BrO2
SMILES: CCCCCCOC(=O)CBr
Mol. weight [g/mol]: 223.11
CAS: 13048-32-3

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	1265.80		NIST Webbook
rinpol	1284.40		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/mol×K	524.89	Joback Method
cpg	332.24	J/mol×K	556.51	Joback Method
cpg	343.62	J/mol×K	588.14	Joback Method
cpg	354.49	J/mol×K	619.76	Joback Method
cpg	364.86	J/mol×K	651.38	Joback Method
cpg	374.73	J/mol×K	683.00	Joback Method

cpg	384.11	J/mol×K	714.63	Joback Method
dvisc	0.0025371	Pa×s	311.88	Joback Method
dvisc	0.0014455	Pa×s	347.38	Joback Method
dvisc	0.0009142	Pa×s	382.88	Joback Method
dvisc	0.0006249	Pa×s	418.38	Joback Method
dvisc	0.0004533	Pa×s	453.89	Joback Method
dvisc	0.0003445	Pa×s	489.39	Joback Method
dvisc	0.0002718	Pa×s	524.89	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=C13048323&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
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

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