

Bromoacetic acid, heptyl ester

Other names:	Heptyl bromoacetate
Inchi:	InChI=1S/C9H17BrO2/c1-2-3-4-5-6-7-12-9(11)8-10/h2-8H2,1H3
InchiKey:	SZZUXOYNCHATNT-UHFFFAOYSA-N
Formula:	C9H17BrO2
SMILES:	CCCCCCCCOC(=O)CBr
Mol. weight [g/mol]:	237.13
CAS:	18991-99-6

Physical Properties

Property code	Value	Unit	Source
gf	-194.70	kJ/mol	Joback Method
hf	-447.56	kJ/mol	Joback Method
hfus	27.14	kJ/mol	Joback Method
hvap	51.22	kJ/mol	Joback Method
log10ws	-2.88		Crippen Method
logp	2.895		Crippen Method
mcvol	162.610	ml/mol	McGowan Method
pc	2584.59	kPa	Joback Method
rinpol	1384.20		NIST Webbook
tb	547.77	K	Joback Method
tc	735.28	K	Joback Method
tf	323.15	K	Joback Method
vc	0.625	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	365.76	J/molxK	547.77	Joback Method
cpg	378.57	J/molxK	579.02	Joback Method
cpg	390.80	J/molxK	610.27	Joback Method
cpg	402.47	J/molxK	641.52	Joback Method
cpg	413.59	J/molxK	672.78	Joback Method
cpg	424.18	J/molxK	704.03	Joback Method
cpg	434.25	J/molxK	735.28	Joback Method

dvisc	0.0024410	Paxs	323.15	Joback Method
dvisc	0.0013642	Paxs	360.59	Joback Method
dvisc	0.0008506	Paxs	398.02	Joback Method
dvisc	0.0005753	Paxs	435.46	Joback Method
dvisc	0.0004139	Paxs	472.90	Joback Method
dvisc	0.0003125	Paxs	510.33	Joback Method
dvisc	0.0002452	Paxs	547.77	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C18991996&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

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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