2- Bromopropionic acid, hexyl ester

Other names:	Hexyl 2-bromopropanoate
	Propanoic acid, 2-bromo, hexyl ester
Inchi:	InChI=1S/C9H17BrO2/c1-3-4-5-6-7-12-9(11)8(2)10/h8H,3-7H2,1-2H3
InchiKey:	CVIVDRZPZOBMDR-UHFFFAOYSA-N
Formula:	C9H17BrO2
SMILES:	CCCCCCOC(=O)C(C)Br
Mol. weight [g/mol]:	237.13
CAS:	28456-82-8

Physical Properties

Property code	Value	Unit	Source
gf	-197.14	kJ/mol	Joback Method
hf	-452.84	kJ/mol	Joback Method
hfus	23.62	kJ/mol	Joback Method
hvap	50.83	kJ/mol	Joback Method
log10ws	-3.00		Crippen Method
logp	2.893		Crippen Method
mcvol	162.610	ml/mol	McGowan Method
pc	2605.74	kPa	Joback Method
rinpol	1298.00		NIST Webbook
rinpol	1328.30		NIST Webbook
rinpol	1328.30		NIST Webbook
rinpol	1312.00		NIST Webbook
rinpol	1292.00		NIST Webbook
rinpol	1298.00		NIST Webbook
ripol	1681.00		NIST Webbook
ripol	1681.00		NIST Webbook
tb	547.33	K	Joback Method
tc	738.62	K	Joback Method
tf	308.15	K	Joback Method
vc	0.620	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	366.10	J/mol×K	547.33	Joback Method
cpg	379.22	J/mol×K	579.21	Joback Method
cpg	391.74	J/mol×K	611.09	Joback Method
cpg	403.67	J/mol×K	642.98	Joback Method
cpg	415.02	J/mol×K	674.86	Joback Method
cpg	425.81	J/mol×K	706.74	Joback Method
cpg	436.04	J/mol×K	738.62	Joback Method
dvisc	0.0031707	Pa×s	308.15	Joback Method
dvisc	0.0015948	Pa×s	348.01	Joback Method
dvisc	0.0009238	Pa×s	387.88	Joback Method
dvisc	0.0005925	Pa×s	427.74	Joback Method
dvisc	0.0004099	Pa×s	467.60	Joback Method
dvisc	0.0003004	Pa×s	507.47	Joback Method
dvisc	0.0002304	Pa×s	547.33	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=C28456828&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
ripol: Polar retention indices

tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume