

6-Bromohexanoic acid, 2,2,2-trichloroethyl ester

Inchi:	InChI=1S/C8H12BrCl3O2/c9-5-3-1-2-4-7(13)14-6-8(10,11)12/h1-6H2
InchiKey:	VMPRRSDTJAASQS-UHFFFAOYSA-N
Formula:	C8H12BrCl3O2
SMILES:	O=C(CCCCCBr)OCC(Cl)(Cl)Cl
Mol. weight [g/mol]:	326.44

Physical Properties

Property code	Value	Unit	Source
gf	-236.07	kJ/mol	Joback Method
hf	-482.89	kJ/mol	Joback Method
hfus	29.73	kJ/mol	Joback Method
hvap	60.85	kJ/mol	Joback Method
log10ws	-4.03		Crippen Method
logp	3.855		Crippen Method
mcvol	185.240	ml/mol	McGowan Method
pc	2595.13	kPa	Joback Method
rinpola	1798.00		NIST Webbook
tb	633.95	K	Joback Method
tc	847.82	K	Joback Method
tf	404.06	K	Joback Method
vc	0.706	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	397.63	J/molxK	633.95	Joback Method
cpg	407.91	J/molxK	669.59	Joback Method
cpg	417.47	J/molxK	705.24	Joback Method
cpg	426.37	J/molxK	740.88	Joback Method
cpg	434.65	J/molxK	776.53	Joback Method
cpg	442.34	J/molxK	812.17	Joback Method
cpg	449.50	J/molxK	847.82	Joback Method
dvisc	0.0016605	Paxs	404.06	Joback Method
dvisc	0.0009777	Paxs	442.38	Joback Method

dvisc	0.0006263	Paxs	480.69	Joback Method
dvisc	0.0004285	Paxs	519.00	Joback Method
dvisc	0.0003089	Paxs	557.32	Joback Method
dvisc	0.0002322	Paxs	595.63	Joback Method
dvisc	0.0001807	Paxs	633.95	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354715&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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