

4-Bromobutyric acid, 8-chlorooctyl ester

Inchi:	InChI=1S/C12H22BrClO2/c13-9-7-8-12(15)16-11-6-4-2-1-3-5-10-14/h1-11H2
InchiKey:	NZSCQBROFMTNGG-UHFFFAOYSA-N
Formula:	C12H22BrClO2
SMILES:	O=C(CCCBr)OCCCCCCCCCl
Mol. weight [g/mol]:	313.66

Physical Properties

Property code	Value	Unit	Source
gf	-181.37	kJ/mol	Joback Method
hf	-525.22	kJ/mol	Joback Method
hfus	39.10	kJ/mol	Joback Method
hvap	62.28	kJ/mol	Joback Method
log10ws	-4.29		Crippen Method
logp	4.284		Crippen Method
mcvol	217.120	ml/mol	McGowan Method
pc	1903.58	kPa	Joback Method
rinpol	2147.00		NIST Webbook
tb	653.84	K	Joback Method
tc	839.99	K	Joback Method
tf	386.88	K	Joback Method
vc	0.843	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	541.86	J/mol×K	653.84	Joback Method
cpg	555.99	J/mol×K	684.86	Joback Method
cpg	569.42	J/mol×K	715.89	Joback Method
cpg	582.17	J/mol×K	746.91	Joback Method
cpg	594.25	J/mol×K	777.94	Joback Method
cpg	605.70	J/mol×K	808.96	Joback Method
cpg	616.53	J/mol×K	839.99	Joback Method
dvisc	0.0017005	Pa×s	386.88	Joback Method
dvisc	0.0009297	Pa×s	431.37	Joback Method

dvisc	0.0005691	Pa×s	475.87	Joback Method
dvisc	0.0003788	Pa×s	520.36	Joback Method
dvisc	0.0002689	Pa×s	564.85	Joback Method
dvisc	0.0002006	Pa×s	609.35	Joback Method
dvisc	0.0001558	Pa×s	653.84	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=U354691&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

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