

6-Bromohexanoic acid, 4-methoxy-2-methylbutyl ester

Inchi:	InChI=1S/C12H23BrO3/c1-11(7-9-15-2)10-16-12(14)6-4-3-5-8-13/h11H,3-10H2,1-2H3
InchiKey:	LBLFFASVIXSIPD-UHFFFAOYSA-N
Formula:	C12H23BrO3
SMILES:	COCCC(C)COC(=O)CCCCBr
Mol. weight [g/mol]:	295.21

Physical Properties

Property code	Value	Unit	Source
gf	-276.88	kJ/mol	Joback Method
hf	-646.98	kJ/mol	Joback Method
hfus	32.57	kJ/mol	Joback Method
hvap	59.92	kJ/mol	Joback Method
log10ws	-2.99		Crippen Method
logp	3.158		Crippen Method
mvol	210.750	ml/mol	McGowan Method
pc	1950.95	kPa	Joback Method
rinpol	1857.00		NIST Webbook
tb	638.39	K	Joback Method
tc	822.58	K	Joback Method
tf	364.19	K	Joback Method
vc	0.805	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	540.11	J/molxK	638.39	Joback Method
cpg	555.09	J/molxK	669.09	Joback Method
cpg	569.38	J/molxK	699.79	Joback Method
cpg	582.97	J/molxK	730.48	Joback Method
cpg	595.89	J/molxK	761.18	Joback Method
cpg	608.14	J/molxK	791.88	Joback Method
cpg	619.72	J/molxK	822.58	Joback Method
dvisc	0.0017819	Paxs	364.19	Joback Method
dvisc	0.0008939	Paxs	409.89	Joback Method

dvisc	0.0005150	Paxs	455.59	Joback Method
dvisc	0.0003281	Paxs	501.29	Joback Method
dvisc	0.0002254	Paxs	546.99	Joback Method
dvisc	0.0001640	Paxs	592.69	Joback Method
dvisc	0.0001250	Paxs	638.39	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=U354716&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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