

4-Bromobutyric acid, 4-methoxy-2-methylbutyl ester

Inchi:	InChI=1S/C10H19BrO3/c1-9(5-7-13-2)8-14-10(12)4-3-6-11/h9H,3-8H2,1-2H3
InchiKey:	OYVOWOWYHJTHDD-UHFFFAOYSA-N
Formula:	C10H19BrO3
SMILES:	COCCC(C)COC(=O)CCBr
Mol. weight [g/mol]:	267.16

Physical Properties

Property code	Value	Unit	Source
gf	-293.72	kJ/mol	Joback Method
hf	-605.70	kJ/mol	Joback Method
hfus	27.39	kJ/mol	Joback Method
hvap	55.47	kJ/mol	Joback Method
log10ws	-2.15		Crippen Method
logp	2.377		Crippen Method
mvol	182.570	ml/mol	McGowan Method
pc	2329.27	kPa	Joback Method
rinpol	1619.00		NIST Webbook
rinpol	1619.00		NIST Webbook
tb	592.63	K	Joback Method
tc	780.39	K	Joback Method
tf	341.65	K	Joback Method
vc	0.694	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	438.95	J/molxK	592.63	Joback Method
cpg	501.43	J/molxK	749.10	Joback Method
cpg	490.13	J/molxK	717.81	Joback Method
cpg	478.24	J/molxK	686.51	Joback Method
cpg	465.75	J/molxK	655.22	Joback Method
cpg	452.65	J/molxK	623.92	Joback Method
cpg	512.12	J/molxK	780.39	Joback Method
dvisc	0.0001609	Paxs	592.63	Joback Method

dvisc	0.0002097	Paxs	550.80	Joback Method
dvisc	0.0002853	Paxs	508.97	Joback Method
dvisc	0.0004103	Paxs	467.14	Joback Method
dvisc	0.0006338	Paxs	425.31	Joback Method
dvisc	0.0010763	Paxs	383.48	Joback Method
dvisc	0.0020810	Paxs	341.65	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354688&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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