

Pentane, 2-bromo-1-methoxy

Inchi:	InChI=1S/C6H13BrO/c1-3-4-6(7)5-8-2/h6H,3-5H2,1-2H3
InchiKey:	FGCPRWSXRZUONP-UHFFFAOYSA-N
Formula:	C6H13BrO
SMILES:	CCCC(Br)COC
Mol. weight [g/mol]:	181.07

Physical Properties

Property code	Value	Unit	Source
gf	-93.48	kJ/mol	Joback Method
hf	-278.34	kJ/mol	Joback Method
hfus	14.25	kJ/mol	Joback Method
hvap	37.41	kJ/mol	Joback Method
log10ws	-1.96		Crippen Method
logp	2.196		Crippen Method
mcvol	118.770	ml/mol	McGowan Method
pc	3325.84	kPa	Joback Method
rinpola	935.00		NIST Webbook
tb	424.82	K	Joback Method
tc	612.54	K	Joback Method
tf	224.41	K	Joback Method
vc	0.446	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	220.06	J/molxK	424.82	Joback Method
cpg	269.61	J/molxK	581.26	Joback Method
cpg	260.50	J/molxK	549.97	Joback Method
cpg	251.00	J/molxK	518.68	Joback Method
cpg	241.10	J/molxK	487.39	Joback Method
cpg	230.79	J/molxK	456.11	Joback Method
cpg	278.33	J/molxK	612.54	Joback Method
dvisc	0.0002837	Paxs	424.82	Joback Method
dvisc	0.0003698	Paxs	391.42	Joback Method

dvisc	0.0005066	Paxs	358.02	Joback Method
dvisc	0.0007403	Paxs	324.62	Joback Method
dvisc	0.0011802	Paxs	291.21	Joback Method
dvisc	0.0021234	Paxs	257.81	Joback Method
dvisc	0.0045501	Paxs	224.41	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R12038&Units=SI

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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