Butane, 2-bromo-3-methoxy, erythro

Inchi: InChI=1S/C5H11BrO/c1-4(6)5(2)7-3/h4-5H,1-3H3/t4-,5+/m1/s1
InchiKey: MNFFVQPIBJUTHA-UHNVWZDZSA-N
Formula: C5H11BrO
SMILES: COC(C)C(C)Br
Mol. weight [g/mol]: 167.04

Physical Properties

Property code	Value	Unit	Source
gf	-104.34	kJ/mol	Joback Method
hf	-262.98	kJ/mol	Joback Method
hfus	8.13	kJ/mol	Joback Method
hvap	34.79	kJ/mol	Joback Method
log10ws	-1.66		Crippen Method
logp	1.805		Crippen Method
mcvol	104.680	ml/mol	McGowan Method
pc	3763.78	kPa	Joback Method
rinpol	818.00		NIST Webbook
rinpol	818.00		NIST Webbook
tb	401.50	K	Joback Method
tc	595.30	K	Joback Method
tf	198.14	K	Joback Method
vc	0.384	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	182.70	J/mol×K	401.50	Joback Method
cpg	227.43	J/mol×K	563.00	Joback Method
cpg	219.22	J/mol×K	530.70	Joback Method
cpg	210.64	J/mol×K	498.40	Joback Method
cpg	201.70	J/mol×K	466.10	Joback Method
cpg	192.39	J/mol×K	433.80	Joback Method
cpg	235.30	J/mol×K	595.30	Joback Method
dvisc	0.0002907	Pa×s	401.50	Joback Method

dvisc	0.0003886	Pa×s	367.61	Joback Method
dvisc	0.0005510	Pa×s	333.71	Joback Method
dvisc	0.0008454	Pa×s	299.82	Joback Method
dvisc	0.0014467	Pa×s	265.93	Joback Method
dvisc	0.0028963	Pa×s	232.03	Joback Method
dvisc	0.0073529	Pa×s	198.14	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R294578&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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