Butane, 2-bromo-3-methyl

Inchi: InChI=1S/C5H11Br/c1-4(2)5(3)6/h4-5H,1-3H3
InchiKey: BLGVDCMNIAOLHA-UHFFFAOYSA-N
Formula: C5H11Br
SMILES: CC(C)C(C)Br
Mol. weight [g/mol]: 151.04

Physical Properties

Property code	Value	Unit	Source
gf	0.66	kJ/mol	Joback Method
hf	-130.76	kJ/mol	Joback Method
hfus	6.95	kJ/mol	Joback Method
hvap	32.38	kJ/mol	Joback Method
log10ws	-2.22		Crippen Method
logp	2.426		Crippen Method
mcvol	98.810	ml/mol	McGowan Method
pc	3843.54	kPa	Joback Method
rinpol	808.00		NIST Webbook
rinpol	808.00		NIST Webbook
ripol	938.00		NIST Webbook
ripol	929.00		NIST Webbook
ripol	951.00		NIST Webbook
ripol	938.00		NIST Webbook
tb	379.08	K	Joback Method
tc	573.07	K	Joback Method
tf	175.91	K	Joback Method
vc	0.365	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	161.24	J/mol×K	379.08	Joback Method
cpg	171.24	J/mol×K	411.41	Joback Method
cpg	180.77	J/mol×K	443.74	Joback Method
cpg	189.84	J/mol×K	476.07	Joback Method

cpg	198.48	J/mol×K	508.41	Joback Method
cpg	206.69	J/mol×K	540.74	Joback Method
cpg	214.50	J/mol×K	573.07	Joback Method
dvisc	0.0109394	Pa×s	175.91	Joback Method
dvisc	0.0038372	Pa×s	209.77	Joback Method
dvisc	0.0018010	Pa×s	243.63	Joback Method
dvisc	0.0010166	Pa×s	277.50	Joback Method
dvisc	0.0006499	Pa×s	311.36	Joback Method
dvisc	0.0004536	Pa×s	345.22	Joback Method
dvisc	0.0003376	Pa×s	379.08	Joback Method

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R91507&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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