

2-Bromo-5-methoxytoluene

Other names:	4-Bromo-3-methylanisole
Inchi:	InChI=1S/C8H9BrO/c1-6-5-7(10-2)3-4-8(6)9/h3-5H,1-2H3
InchiKey:	BLZNSXFQRKVFRP-UHFFFAOYSA-N
Formula:	C8H9BrO
SMILES:	COc1ccc(Br)c(C)c1
Mol. weight [g/mol]:	201.06
CAS:	27060-75-9

Physical Properties

Property code	Value	Unit	Source
gf	18.95	kJ/mol	Joback Method
hf	-100.75	kJ/mol	Joback Method
hfus	16.21	kJ/mol	Joback Method
hvap	45.85	kJ/mol	Joback Method
log10ws	-3.23		Crippen Method
logp	2.766		Crippen Method
mcvol	123.190	ml/mol	McGowan Method
pc	3749.97	kPa	Joback Method
tb	507.66	K	Joback Method
tc	736.20	K	Joback Method
tf	313.41	K	Joback Method
vc	0.456	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	234.41	J/molxK	507.66	Joback Method
cpg	283.84	J/molxK	698.11	Joback Method
cpg	275.10	J/molxK	660.02	Joback Method
cpg	265.79	J/molxK	621.93	Joback Method
cpg	255.92	J/molxK	583.84	Joback Method
cpg	245.46	J/molxK	545.75	Joback Method
cpg	292.05	J/molxK	736.20	Joback Method
dvisc	0.0002318	Paxs	507.66	Joback Method

dvisc	0.0002797	Paxs	475.28	Joback Method
dvisc	0.0003470	Paxs	442.91	Joback Method
dvisc	0.0004454	Paxs	410.53	Joback Method
dvisc	0.0005966	Paxs	378.16	Joback Method
dvisc	0.0008440	Paxs	345.78	Joback Method
dvisc	0.0012829	Paxs	313.41	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C27060759&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

cp_g:	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
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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