Dimethyl 5-bromoisophthalate

Other names: dimethyl 5-bromoisophthalate
Inchi: InChI=1S/C10H9BrO4/c1-14-9(12)6-3-7(10(13)15-2)5-8(11)4-6/h3-5H,1-2H3
InchiKey: QUJINGKSNJNXEB-UHFFFAOYSA-N
Formula: C10H9BrO4
SMILES: COC(=O)c1cc(Br)cc(C(=O)OC)c1
Mol. weight [g/mol]: 273.08

Physical Properties

Property code	Value	Unit	Source
af	0.6479		Cheméo Relay (1.0)
hf	-595.28	kJ/mol	Cheméo Relay (1.0)
hfus	25.78	kJ/mol	Joback Method
hvap	78.30	kJ/mol	Cheméo Relay (1.0)
ie	9.60	eV	Cheméo Relay (1.0)
log10ws	-4.03		Cheméo Relay (1.0)
logp	2.022		Crippen Method
mcvol	160.380	ml/mol	McGowan Method
pc	3395.98	kPa	Joback Method
tb	578.05	K	Cheméo Relay (1.0)
tc	786.32	K	Cheméo Relay (1.0)
tf	390.20	K	Cheméo Relay (1.0)
vc	0.578	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	370.20	J/mol×K	683.58	Joback Method
cpg	380.78	J/mol×K	722.13	Joback Method
cpg	390.61	J/mol×K	760.69	Joback Method
cpg	399.69	J/mol×K	799.24	Joback Method
cpg	408.03	J/mol×K	837.79	Joback Method
cpg	415.60	J/mol×K	876.35	Joback Method
cpg	422.41	J/mol×K	914.90	Joback Method
dvisc	0.0008269	Pa×s	458.04	Joback Method

dvisc	0.0005740	Pa×s	495.63	Joback Method
dvisc	0.0004196	Pa×s	533.22	Joback Method
dvisc	0.0003196	Pa×s	570.81	Joback Method
dvisc	0.0002517	Pa×s	608.40	Joback Method
dvisc	0.0002039	Pa×s	645.99	Joback Method
dvisc	0.0001690	Pa×s	683.58	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C51760215&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af: Acentric Factor
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: 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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.