P-(2-BROMOETHYL)BENZOIC ACID

Other names: p-(«beta»-Bromoethyl)benzoic acid
p-(b-Bromoethyl)benzoic acid
Benzoic acid, 4-(2-bromoethyl)-
4-(2-bromoethyl)benzoic acid
Inchi: InChI=1S/C9H9BrO2/c10-6-5-7-1-3-8(4-2-7)9(11)12/h1-4H,5-6H2,(H,11,12)
InchiKey: BKMRWJWLBHHGCF-UHFFFAOYSA-N
Formula: C9H9BrO2
SMILES: O=C(O)c1ccc(CCBr)cc1
Mol. weight [g/mol]: 229.07

Physical Properties

Property code	Value	Unit	Source
af	0.7872		Cheméo Relay (1.0)
gf	-123.74	kJ/mol	Joback Method
hf	-334.80	kJ/mol	Cheméo Relay (1.0)
hfus	23.69	kJ/mol	Joback Method
hvap	101.87	kJ/mol	Cheméo Relay (1.0)
ie	9.44	eV	Cheméo Relay (1.0)
log10ws	-3.22		Cheméo Relay (1.0)
logp	2.322		Crippen Method
mcvol	138.850	ml/mol	McGowan Method
pc	4205.63	kPa	Joback Method
tb	589.35	K	Cheméo Relay (1.0)
tc	820.82	K	Cheméo Relay (1.0)
tf	438.68	K	Cheméo Relay (1.0)
vc	0.470	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	312.02	J/mol×K	649.19	Joback Method
cpg	321.22	J/mol×K	685.20	Joback Method
cpg	329.79	J/mol×K	721.21	Joback Method
cpg	337.77	J/mol×K	757.22	Joback Method

cpg	345.18	J/mol×K	793.23	Joback Method
cpg	352.08	J/mol×K	829.24	Joback Method
cpg	358.50	J/mol×K	865.25	Joback Method
dvisc	0.0021704	Pa×s	400.68	Joback Method
dvisc	0.0009823	Pa×s	442.10	Joback Method
dvisc	0.0005092	Pa×s	483.52	Joback Method
dvisc	0.0002928	Pa×s	524.94	Joback Method
dvisc	0.0001826	Pa×s	566.35	Joback Method
dvisc	0.0001214	Pa×s	607.77	Joback Method
dvisc	0.0000851	Pa×s	649.19	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C52062927&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

Legend

af: Acentric Factor
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
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