4'-(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
CAS:	52062-92-7

Physical Properties

Property code	Value	Unit	Source
gf	-123.74	kJ/mol	Joback Method
hf	-242.51	kJ/mol	Joback Method
hfus	23.69	kJ/mol	Joback Method
hvap	68.43	kJ/mol	Joback Method
log10ws	-2.77		Crippen Method
logp	2.322		Crippen Method
mcvol	138.850	ml/mol	McGowan Method
pc	4205.63	kPa	Joback Method
tb	649.19	K	Joback Method
tc	865.25	K	Joback Method
tf	400.68	K	Joback Method
vc	0.518	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	312.02	J/mol×K	649.19	Joback Method
cpg	352.08	J/mol×K	829.24	Joback Method
cpg	345.18	J/mol×K	793.23	Joback Method
cpg	337.77	J/mol×K	757.22	Joback Method
cpg	329.79	J/mol×K	721.21	Joback Method

cpg	321.22	J/mol×K	685.20	Joback Method
cpg	358.50	J/mol×K	865.25	Joback Method
dvisc	0.0000851	Pa×s	649.19	Joback Method
dvisc	0.0001214	Pa×s	607.77	Joback Method
dvisc	0.0001826	Pa×s	566.35	Joback Method
dvisc	0.0002928	Pa×s	524.94	Joback Method
dvisc	0.0005092	Pa×s	483.52	Joback Method
dvisc	0.0009823	Pa×s	442.10	Joback Method
dvisc	0.0021704	Pa×s	400.68	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C52062927&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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