O-bromophenetole

Other names: 2-bromophenetole
Inchi: InChI=1S/C8H9BrO/c1-2-10-8-6-4-3-5-7(8)9/h3-6H,2H2,1H3
InchiKey: JVEQWIQHHWNMQX-UHFFFAOYSA-N
Formula: C8H9BrO
SMILES: CCOc1ccccc1Br
Mol. weight [g/mol]: 201.06
CAS: 583-19-7

Physical Properties

Property code	Value	Unit	Source
gf	28.58	kJ/mol	Joback Method
hf	-89.28	kJ/mol	Joback Method
hfus	16.60	kJ/mol	Joback Method
hvap	45.19	kJ/mol	Joback Method
log10ws	-3.17		Crippen Method
logp	2.848		Crippen Method
mcvol	123.190	ml/mol	McGowan Method
pc	3819.82	kPa	Joback Method
rinpol	1225.60		NIST Webbook
tb	502.68	K	Joback Method
tc	729.96	K	Joback Method
tf	300.89	K	Joback Method
vc	0.456	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	234.74	J/mol×K	502.68	Joback Method
cpg	285.51	J/mol×K	692.08	Joback Method
cpg	276.60	J/mol×K	654.20	Joback Method
cpg	267.10	J/mol×K	616.32	Joback Method
cpg	256.97	J/mol×K	578.44	Joback Method
cpg	246.19	J/mol×K	540.56	Joback Method
cpg	293.82	J/mol×K	729.96	Joback Method

dvisc	0.0002401	Pa×s	502.68	Joback Method
dvisc	0.0002954	Pa×s	469.05	Joback Method
dvisc	0.0003752	Pa×s	435.42	Joback Method
dvisc	0.0004961	Pa×s	401.78	Joback Method
dvisc	0.0006903	Pa×s	368.15	Joback Method
dvisc	0.0010265	Pa×s	334.52	Joback Method
dvisc	0.0016679	Pa×s	300.89	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C583197&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

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