

Benzoic acid, (2-bromophenyl)methyl ester

Inchi:	InChI=1S/C14H11BrO2/c15-13-9-5-4-8-12(13)10-17-14(16)11-6-2-1-3-7-11/h1-9H,10H2
InchiKey:	DETHHGJSHHWELU-UHFFFAOYSA-N
Formula:	C14H11BrO2
SMILES:	O=C(OCc1ccccc1Br)c1ccccc1
Mol. weight [g/mol]:	291.14

Physical Properties

Property code	Value	Unit	Source
gf	62.59	kJ/mol	Joback Method
hf	-89.17	kJ/mol	Joback Method
hfus	27.78	kJ/mol	Joback Method
hvap	67.56	kJ/mol	Joback Method
log10ws	-4.99		Crippen Method
logp	3.806		Crippen Method
mcvol	185.540	ml/mol	McGowan Method
pc	3086.42	kPa	Joback Method
rinsol	2108.00		NIST Webbook
tb	720.51	K	Joback Method
tc	974.88	K	Joback Method
tf	444.86	K	Joback Method
vc	0.690	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	450.38	J/molxK	720.51	Joback Method
cpg	463.65	J/molxK	762.90	Joback Method
cpg	475.74	J/molxK	805.30	Joback Method
cpg	486.72	J/molxK	847.69	Joback Method
cpg	496.67	J/molxK	890.09	Joback Method
cpg	505.64	J/molxK	932.48	Joback Method
cpg	513.71	J/molxK	974.88	Joback Method
dvisc	0.0009888	Paxs	444.86	Joback Method
dvisc	0.0006098	Paxs	490.80	Joback Method

dvisc	0.0004085	Paxs	536.74	Joback Method
dvisc	0.0002915	Paxs	582.68	Joback Method
dvisc	0.0002185	Paxs	628.63	Joback Method
dvisc	0.0001704	Paxs	674.57	Joback Method
dvisc	0.0001371	Paxs	720.51	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U368715&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

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

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