

Formic acid, (3-bromophenyl)methyl ester

Inchi:	InChI=1S/C8H7BrO2/c9-8-3-1-2-7(4-8)5-11-6-10/h1-4,6H,5H2
InchiKey:	DHMOFWPIPCIXNL-UHFFFAOYSA-N
Formula:	C8H7BrO2
SMILES:	O=COCc1cccc(Br)c1
Mol. weight [g/mol]:	215.04

Physical Properties

Property code	Value	Unit	Source
gf	-70.94	kJ/mol	Joback Method
hf	-174.86	kJ/mol	Joback Method
hfus	18.89	kJ/mol	Joback Method
hvap	51.91	kJ/mol	Joback Method
log10ws	-2.79		Crippen Method
logp	2.122		Crippen Method
mcvol	124.760	ml/mol	McGowan Method
pc	4194.74	kPa	Joback Method
rinsol	1375.00		NIST Webbook
tb	551.34	K	Joback Method
tc	781.91	K	Joback Method
tf	342.89	K	Joback Method
vc	0.472	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	248.43	J/molxK	551.34	Joback Method
cpg	258.42	J/molxK	589.77	Joback Method
cpg	267.75	J/molxK	628.20	Joback Method
cpg	276.47	J/molxK	666.63	Joback Method
cpg	284.57	J/molxK	705.06	Joback Method
cpg	292.09	J/molxK	743.48	Joback Method
cpg	299.04	J/molxK	781.91	Joback Method
dvisc	0.0017422	Paxs	342.89	Joback Method
dvisc	0.0011204	Paxs	377.63	Joback Method

dvisc	0.0007762	Paxs	412.37	Joback Method
dvisc	0.0005693	Paxs	447.12	Joback Method
dvisc	0.0004366	Paxs	481.86	Joback Method
dvisc	0.0003470	Paxs	516.60	Joback Method
dvisc	0.0002839	Paxs	551.34	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U368725&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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