3-Bromobenzoic acid. 3-methylbut-2-enyl ester

Inchi: InChI=1S/C12H13BrO2/c1-9(2)6-7-15-12(14)10-4-3-5-11(13)8-10/h3-6,8H,7H2,1-2H3
InchiKey: SCHFXORPCOMCOF-UHFFFAOYSA-N
Formula: C12H13BrO2
SMILES: CC(C)=CCOC(=O)c1cccc(Br)c1
Mol. weight [g/mol]: 269.13

Physical Properties

Property code	Value	Unit	Source
gf	5.01	kJ/mol	Joback Method
hf	-176.99	kJ/mol	Joback Method
hfus	27.45	kJ/mol	Joback Method
hvap	60.87	kJ/mol	Joback Method
log10ws	-4.40		Crippen Method
logp	3.572		Crippen Method
mcvol	176.820	ml/mol	McGowan Method
pc	2823.32	kPa	Joback Method
rinpol	1714.00		NIST Webbook
rinpol	1714.00		NIST Webbook
tb	652.11	K	Joback Method
tc	884.01	K	Joback Method
tf	376.86	K	Joback Method
vc	0.666	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	411.62	J/mol×K	652.11	Joback Method
cpg	424.90	J/mol×K	690.76	Joback Method
cpg	437.27	J/mol×K	729.41	Joback Method
cpg	448.77	J/mol×K	768.06	Joback Method
cpg	459.46	J/mol×K	806.71	Joback Method
cpg	469.39	J/mol×K	845.36	Joback Method
cpg	478.62	J/mol×K	884.01	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299140&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
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