3-Bromobenzoic acid, oct-3-en-2-yl ester

Inchi: InChI=1S/C15H19BrO2/c1-3-4-5-6-8-12(2)18-15(17)13-9-7-10-14(16)11-13/h6-12H,3-5H
InchiKey: UOEBIVUSZSTAHC-SOFGYWHQSA-N
Formula: C15H19BrO2
SMILES: CCCCC=CC(C)OC(=O)c1cccc(Br)c1
Mol. weight [g/mol]: 311.21

Physical Properties

Property code	Value	Unit	Source
gf	36.38	kJ/mol	Joback Method
hf	-234.40	kJ/mol	Joback Method
hfus	33.01	kJ/mol	Joback Method
hvap	67.08	kJ/mol	Joback Method
log10ws	-5.77		Crippen Method
logp	4.741		Crippen Method
mcvol	219.090	ml/mol	McGowan Method
pc	2129.52	kPa	Joback Method
rinpol	1915.00		NIST Webbook
rinpol	1915.00		NIST Webbook
tb	720.43	K	Joback Method
tc	940.78	K	Joback Method
tf	409.63	K	Joback Method
vc	0.828	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	566.72	J/mol×K	720.43	Joback Method
cpg	632.06	J/mol×K	904.06	Joback Method
cpg	620.74	J/mol×K	867.33	Joback Method
cpg	608.60	J/mol×K	830.61	Joback Method
cpg	595.59	J/mol×K	793.88	Joback Method
cpg	581.64	J/mol×K	757.16	Joback Method
cpg	642.62	J/mol×K	940.78	Joback Method
dvisc	0.0000953	Pa×s	720.43	Joback Method

dvisc	0.0001229	Pa×s	668.63	Joback Method
dvisc	0.0001656	Pa×s	616.83	Joback Method
dvisc	0.0002356	Pa×s	565.03	Joback Method
dvisc	0.0003599	Pa×s	513.23	Joback Method
dvisc	0.0006047	Pa×s	461.43	Joback Method
dvisc	0.0011585	Pa×s	409.63	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299143&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