

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

Inchi:	InChI=1S/C15H19BrO2/c1-3-4-5-6-9-12(2)18-15(17)13-10-7-8-11-14(13)16/h6-12H,3-5H
InchiKey:	FKFCDRGNCLBOLW-RMKNXTFCSA-N
Formula:	C15H19BrO2
SMILES:	CCCCC=CC(C)OC(=O)c1ccccc1Br
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	1911.00		NIST Webbook
rinpol	1911.00		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/molxK	720.43	Joback Method
cpg	581.64	J/molxK	757.16	Joback Method
cpg	595.59	J/molxK	793.88	Joback Method
cpg	608.60	J/molxK	830.61	Joback Method
cpg	620.74	J/molxK	867.33	Joback Method
cpg	632.06	J/molxK	904.06	Joback Method
cpg	642.62	J/molxK	940.78	Joback Method
dvisc	0.0011585	Paxs	409.63	Joback Method

dvisc	0.0006047	Paxs	461.43	Joback Method
dvisc	0.0003599	Paxs	513.23	Joback Method
dvisc	0.0002356	Paxs	565.03	Joback Method
dvisc	0.0001656	Paxs	616.83	Joback Method
dvisc	0.0001229	Paxs	668.63	Joback Method
dvisc	0.0000953	Paxs	720.43	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299395&Units=SI

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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