2-Bromobenzoic acid, 2-naphthyl ester

Inchi: InChI=1S/C17H11BrO2/c18-16-8-4-3-7-15(16)17(19)20-14-10-9-12-5-1-2-6-13(12)11-14/
InchiKey: HNTXBLZKNZXOPY-UHFFFAOYSA-N
Formula: C17H11BrO2
SMILES: O=C(Oc1ccc2ccccc2c1)c1ccccc1Br
Mol. weight [g/mol]: 327.17

Physical Properties

Property code	Value	Unit	Source
gf	184.87	kJ/mol	Joback Method
hf	28.51	kJ/mol	Joback Method
hfus	32.18	kJ/mol	Joback Method
hvap	76.54	kJ/mol	Joback Method
log10ws	-6.53		Crippen Method
logp	4.822		Crippen Method
mcvol	208.350	ml/mol	McGowan Method
pc	2896.73	kPa	Joback Method
rinpol	2520.00		NIST Webbook
rinpol	2520.00		NIST Webbook
tb	813.11	K	Joback Method
tc	1079.90	K	Joback Method
tf	523.89	K	Joback Method
vc	0.779	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	533.76	J/mol×K	813.11	Joback Method
cpg	585.95	J/mol×K	1035.44	Joback Method
cpg	577.22	J/mol×K	990.97	Joback Method
cpg	567.77	J/mol×K	946.51	Joback Method
cpg	557.45	J/mol×K	902.04	Joback Method
cpg	546.16	J/mol×K	857.58	Joback Method
cpg	594.09	J/mol×K	1079.90	Joback Method
dvisc	0.0001834	Pa×s	813.11	Joback Method

dvisc	0.0002180	Pa×s	764.91	Joback Method
dvisc	0.0002653	Pa×s	716.70	Joback Method
dvisc	0.0003321	Pa×s	668.50	Joback Method
dvisc	0.0004304	Pa×s	620.30	Joback Method
dvisc	0.0005827	Pa×s	572.09	Joback Method
dvisc	0.0008342	Pa×s	523.89	Joback Method

Sources

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=U307749&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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