2-BROMOFLUORENE

Other names: 2-bromo-9H-fluorene
Inchi: InChI=1S/C13H9Br/c14-11-5-6-13-10(8-11)7-9-3-1-2-4-12(9)13/h1-6,8H,7H2
InchiKey: FXSCJZNMWILAJO-UHFFFAOYSA-N
Formula: C13H9Br
SMILES: Brc1ccc2c(c1)Cc1ccccc1-2
Mol. weight [g/mol]: 245.12

Physical Properties

Property code	Value	Unit	Source
hf	228.82	kJ/mol	Cheméo Relay (1.0)
hfus	17.02	kJ/mol	Thermodynamic properties of bromine fluorene derivatives: An experimental and computational study
hvap	83.83	kJ/mol	Cheméo Relay (1.0)
ie	8.12	eV	Cheméo Relay (1.0)
log10ws	-6.21		Cheméo Relay (1.0)
logp	4.020		Crippen Method
mcvol	153.150	ml/mol	McGowan Method
tb	628.45	K	Cheméo Relay (1.0)
tc	874.34	K	Cheméo Relay (1.0)
tf	376.26	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	340.74	J/mol×K	634.17	Joback Method
cpg	353.24	J/mol×K	677.82	Joback Method
cpg	364.63	J/mol×K	721.48	Joback Method
cpg	375.09	J/mol×K	765.13	Joback Method
cpg	384.77	J/mol×K	808.78	Joback Method
cpg	393.86	J/mol×K	852.44	Joback Method
cpg	402.53	J/mol×K	896.09	Joback Method
dvisc	0.0016708	Pa×s	415.69	Joback Method

dvisc	0.0013665	Pa×s	452.10	Joback Method
dvisc	0.0011517	Pa×s	488.52	Joback Method
dvisc	0.0009939	Pa×s	524.93	Joback Method
dvisc	0.0008743	Pa×s	561.34	Joback Method
dvisc	0.0007812	Pa×s	597.76	Joback Method
dvisc	0.0007071	Pa×s	634.17	Joback Method

Sources

Thermodynamic properties of bromine fluorene derivatives: An experimental and computational study:	https://www.doi.org/10.1016/j.jct.2015.05.001
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1133808&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0, beta):	
Determination of sublimation enthalpies of substituted benzophenones, fluorenes and diphenyl ethers by solution calorimetry approach:	https://www.doi.org/10.1016/j.tca.2017.08.003
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Cheméo Relay (1.0):	

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point