9-Bromofluorene

Other names: 9-Bromofluorene
Fluorene, 9-bromo-
Inchi: InChI=1S/C13H9Br/c14-13-11-7-3-1-5-9(11)10-6-2-4-8-12(10)13/h1-8,13H
InchiKey: AHCDKANCCBEQJJ-UHFFFAOYSA-N
Formula: C13H9Br
SMILES: BrC1c2ccccc2-c2ccccc21
Mol. weight [g/mol]: 245.12

Physical Properties

Property code	Value	Unit	Source
hf	193.19	kJ/mol	Cheméo Relay (1.0)
hfus	24.35	kJ/mol	Joback Method
hvap	79.36	kJ/mol	Cheméo Relay (1.0)
ie	8.26	eV	Cheméo Relay (1.0)
logp	4.151		Crippen Method
mcvol	153.150	ml/mol	McGowan Method
tf	432.09	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	344.72	J/mol×K	624.52	Joback Method
cpg	358.05	J/mol×K	668.05	Joback Method
cpg	370.18	J/mol×K	711.58	Joback Method
cpg	381.26	J/mol×K	755.11	Joback Method
cpg	391.47	J/mol×K	798.64	Joback Method
cpg	400.97	J/mol×K	842.17	Joback Method
cpg	409.94	J/mol×K	885.70	Joback Method
dvisc	0.0017520	Pa×s	398.93	Joback Method
dvisc	0.0014610	Pa×s	436.53	Joback Method
dvisc	0.0012540	Pa×s	474.13	Joback Method
dvisc	0.0011008	Pa×s	511.73	Joback Method
dvisc	0.0009837	Pa×s	549.32	Joback Method
dvisc	0.0008918	Pa×s	586.92	Joback Method

dvisc	0.0008181	Pa×s	624.52	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1940574&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point

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