Fluoren-9-one, 3-bromo-

Inchi: InChI=1S/C13H7BrO/c14-8-5-6-11-12(7-8)9-3-1-2-4-10(9)13(11)15/h1-7H
InchiKey: XWRAQISPRVFAQK-UHFFFAOYSA-N
Formula: C13H7BrO
SMILES: O=C1c2ccccc2-c2cc(Br)ccc21
Mol. weight [g/mol]: 259.10
CAS: 2041-19-2

Physical Properties

Property code	Value	Unit	Source
gf	238.90	kJ/mol	Joback Method
hf	121.09	kJ/mol	Joback Method
hfus	22.40	kJ/mol	Joback Method
hvap	61.63	kJ/mol	Joback Method
log10ws	-5.44		Crippen Method
logp	3.660		Crippen Method
mcvol	154.720	ml/mol	McGowan Method
pc	3754.57	kPa	Joback Method
tb	701.99	K	Joback Method
tc	975.63	K	Joback Method
tf	483.91	K	Joback Method
vc	0.591	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	359.11	J/mol×K	701.99	Joback Method
cpg	370.76	J/mol×K	747.60	Joback Method
cpg	381.45	J/mol×K	793.20	Joback Method
cpg	391.32	J/mol×K	838.81	Joback Method
cpg	400.51	J/mol×K	884.42	Joback Method
cpg	409.13	J/mol×K	930.02	Joback Method
cpg	417.32	J/mol×K	975.63	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2041192&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume