9-Bromo triptycene

Other names: 9,10[1',2']-Benzenoanthracene, 9-bromo-9,10-dihydro-
Inchi: InChI=1S/C20H13Br/c21-20-16-10-4-1-7-13(16)19(14-8-2-5-11-17(14)20)15-9-3-6-12-18
InchiKey: HSROKCVTEYMWHO-UHFFFAOYSA-N
Formula: C20H13Br
SMILES: BrC12c3ccccc3C(c3ccccc31)c1ccccc12
Mol. weight [g/mol]: 333.22
CAS: 15364-55-3

Physical Properties

Property code	Value	Unit	Source
gf	604.59	kJ/mol	Joback Method
hf	430.86	kJ/mol	Joback Method
hfus	32.17	kJ/mol	Joback Method
hvap	73.35	kJ/mol	Joback Method
ie	8.04	eV	NIST Webbook
ie	7.90	eV	NIST Webbook
log10ws	-6.16		Crippen Method
logp	5.180		Crippen Method
mcvol	217.160	ml/mol	McGowan Method
pc	2724.01	kPa	Joback Method
tb	814.78	K	Joback Method
tc	1094.16	K	Joback Method
tf	565.64	K	Joback Method
vc	0.838	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	586.86	J/mol×K	814.78	Joback Method
cpg	602.97	J/mol×K	861.34	Joback Method
cpg	619.46	J/mol×K	907.91	Joback Method
cpg	636.84	J/mol×K	954.47	Joback Method
cpg	655.65	J/mol×K	1001.04	Joback Method
cpg	676.42	J/mol×K	1047.60	Joback Method

cpg	699.69	J/mol×K	1094.16	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C15364553&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

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
ie:	Ionization energy
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