1-AMINO-4-BROMO-2-METHYLANTHRAQUINONE

Other names: Anthraquinone, 1-amino-4-bromo-2-methyl-
1-Amino-4-bromo-2-methylanthraquinone
1-Amino-2-methyl-4-bromoanthraquinone
Inchi: InChI=1S/C15H10BrNO2/c1-7-6-10(16)11-12(13(7)17)15(19)9-5-3-2-4-8(9)14(11)18/h2-6
InchiKey: VIQMJMDPUIBXQO-UHFFFAOYSA-N
Formula: C15H10BrNO2
SMILES: Cc1cc(Br)c2c(c1N)C(=O)c1ccccc1C2=O
Mol. weight [g/mol]: 316.15

Physical Properties

Property code	Value	Unit	Source
hfus	29.41	kJ/mol	Joback Method
ie	8.05	eV	Cheméo Relay (1.0)
logp	3.115		Crippen Method
mcvol	194.450	ml/mol	McGowan Method
tf	479.74	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	533.63	J/mol×K	902.33	Joback Method
cpg	544.77	J/mol×K	949.16	Joback Method
cpg	554.74	J/mol×K	995.98	Joback Method
cpg	563.57	J/mol×K	1042.81	Joback Method
cpg	571.32	J/mol×K	1089.63	Joback Method
cpg	578.02	J/mol×K	1136.46	Joback Method
cpg	583.71	J/mol×K	1183.28	Joback Method

Sources

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):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C81505&Units=SI
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
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point