1-Amino-5-benzamidoanthraquinone

Other names: N-(5-amino-9,10-dihydro-9,10-dioxo-1-anthryl)benzamide
Inchi: InChI=1S/C21H14N2O3/c22-15-10-4-8-13-17(15)19(24)14-9-5-11-16(18(14)20(13)25)23
InchiKey: FWEQPMZEKHHFTB-UHFFFAOYSA-N
Formula: C21H14N2O3
SMILES: Nc1cccc2c1C(=O)c1cccc(NC(=O)c3ccccc3)c1C2=O
Mol. weight [g/mol]: 342.35
CAS: 117-06-6

Physical Properties

Property code	Value	Unit	Source
gf	286.95	kJ/mol	Joback Method
hf	-14.48	kJ/mol	Joback Method
hfus	40.79	kJ/mol	Joback Method
hvap	104.18	kJ/mol	Joback Method
log10ws	-5.24		Crippen Method
logp	3.296		Crippen Method
mcvol	249.280	ml/mol	McGowan Method
pc	2603.08	kPa	Joback Method
tb	1099.19	K	Joback Method
tc	1380.57	K	Joback Method
tf	803.76	K	Joback Method
vc	0.938	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	788.75	J/mol×K	1099.19	Joback Method
cpg	797.00	J/mol×K	1146.09	Joback Method
cpg	803.93	J/mol×K	1192.98	Joback Method
cpg	809.62	J/mol×K	1239.88	Joback Method
cpg	814.18	J/mol×K	1286.78	Joback Method
cpg	817.69	J/mol×K	1333.67	Joback Method
cpg	820.27	J/mol×K	1380.57	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C117066&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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