Benzo[lmn][3,8]phenanthroline-1,3,6,8(2H,7H)-tetr

Other names:	1,4,5,8-Naphthalenetetracarboxylic 1,8: 4,5-diimide naphthalene-1,8:4,5-tetracarboxydiimide
Inchi:	InChI=1S/C14H6N2O4/c17-11-5-1-2-6-10-8(14(20)16-12(6)18)4-3-7(9(5)10)13(19)15-11/
InchiKey:	BODUWJSFPLUDMP-UHFFFAOYSA-N
Formula:	C14H6N2O4
SMILES:	O=C1NC(=O)c2ccc3c4c(ccc1c24)C(=O)NC3=O
Mol. weight [g/mol]:	266.21
CAS:	5690-24-4

Physical Properties

Property code	Value	Unit	Source
gf	69.52	kJ/mol	Joback Method
hf	-239.47	kJ/mol	Joback Method
hfus	32.87	kJ/mol	Joback Method
hvap	84.27	kJ/mol	Joback Method
log10ws	-4.39		Crippen Method
logp	0.607		Crippen Method
mcvol	169.420	ml/mol	McGowan Method
pc	4271.86	kPa	Joback Method
tb	976.50	K	Joback Method
tc	1273.98	K	Joback Method
tf	884.04	K	Joback Method
vc	0.651	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	520.72	J/mol×K	976.50	Joback Method
cpg	529.77	J/mol×K	1026.08	Joback Method
cpg	536.86	J/mol×K	1075.66	Joback Method
cpg	541.90	J/mol×K	1125.24	Joback Method
cpg	544.82	J/mol×K	1174.82	Joback Method
cpg	545.56	J/mol×K	1224.40	Joback Method
cpg	544.03	J/mol×K	1273.98	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5690244&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

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