1,2-Naphthalenedione, 4-(phenylamino)-

Other names: 1,2-Naphthoquinone, 4-anilino-,
Inchi: InChI=1S/C16H11NO2/c18-15-10-14(17-11-6-2-1-3-7-11)12-8-4-5-9-13(12)16(15)19/h1-
InchiKey: NMSRYZBDOYDJBJ-UHFFFAOYSA-N
Formula: C16H11NO2
SMILES: O=C1C=C(Nc2ccccc2)c2ccccc2C1=O
Mol. weight [g/mol]: 249.26
CAS: 27828-56-4

Physical Properties

Property code	Value	Unit	Source
gf	219.93	kJ/mol	Joback Method
hf	-0.62	kJ/mol	Joback Method
hfus	24.81	kJ/mol	Joback Method
hvap	72.70	kJ/mol	Joback Method
log10ws	-3.86		Crippen Method
logp	2.905		Crippen Method
mcvol	186.740	ml/mol	McGowan Method
pc	3035.62	kPa	Joback Method
tb	829.45	K	Joback Method
tc	1104.82	K	Joback Method
tf	556.48	K	Joback Method
vc	0.701	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	536.62	J/mol×K	829.45	Joback Method
cpg	550.52	J/mol×K	875.34	Joback Method
cpg	562.83	J/mol×K	921.24	Joback Method
cpg	573.59	J/mol×K	967.13	Joback Method
cpg	582.83	J/mol×K	1013.03	Joback Method
cpg	590.61	J/mol×K	1058.92	Joback Method
cpg	596.96	J/mol×K	1104.82	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C27828564&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