

Tetraphenylnaphthacene monoxide

Inchi:	InChI=1S/C42H28O/c1-5-17-29(18-6-1)37-33-25-13-14-26-34(33)38(30-19-7-2-8-20-30)
InchiKey:	RHSJHTZJVINNOH-UHFFFAOYSA-N
Formula:	C42H28O
SMILES:	<chem>c1ccc(-c2c3c(c(-c4ccccc4)c4ccccc24)C2(c4ccccc4)OC3(c3ccccc3)c3ccccc32)cc1</chem>
Mol. weight [g/mol]:	548.67
CAS:	127257-80-1

Physical Properties

Property code	Value	Unit	Source
gf	1096.42	kJ/mol	Joback Method
hf	705.25	kJ/mol	Joback Method
hfus	61.81	kJ/mol	Joback Method
hvap	129.21	kJ/mol	Joback Method
log10ws	-13.68		Crippen Method
logp	10.101		Crippen Method
mcvol	424.770	ml/mol	McGowan Method
pc	1250.38	kPa	Joback Method
tb	1392.42	K	Joback Method
tc	1713.06	K	Joback Method
tf	937.73	K	Joback Method
vc	1.617	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1839.98	J/molxK	1392.42	Joback Method
cpg	1948.03	J/molxK	1445.86	Joback Method
cpg	2070.43	J/molxK	1499.30	Joback Method
cpg	2208.53	J/molxK	1552.74	Joback Method
cpg	2363.67	J/molxK	1606.18	Joback Method
cpg	2537.21	J/molxK	1659.62	Joback Method
cpg	2730.50	J/molxK	1713.06	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C127257801&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
h vap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m cvol:	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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