

Heptaphene

Inchi:	InChI=1S/C30H18/c1-3-7-21-13-27-17-29-23(15-25(27)11-19(21)5-1)9-10-24-16-26-12-2
InchiKey:	ACJRMEVDTSKFDP-UHFFFAOYSA-N
Formula:	C30H18
SMILES:	<chem>c1ccc2cc3cc4c(ccc5cc6cc7ccccc7cc6cc54)cc3cc2c1</chem>
Mol. weight [g/mol]:	378.46
CAS:	222-75-3

Physical Properties

Property code	Value	Unit	Source
gf	905.88	kJ/mol	Joback Method
hf	663.07	kJ/mol	Joback Method
hfus	47.67	kJ/mol	Joback Method
hvap	97.80	kJ/mol	Joback Method
ie	6.89 ± 0.02	eV	NIST Webbook
ie	6.98 ± 0.04	eV	NIST Webbook
log10ws	-12.30		Crippen Method
logp	8.606		Crippen Method
mcvol	293.040	ml/mol	McGowan Method
pc	1777.34	kPa	Joback Method
tb	1051.26	K	Joback Method
tc	1330.47	K	Joback Method
tf	713.08	K	Joback Method
vc	1.139	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	909.76	J/mol×K	1051.26	Joback Method
cpg	929.78	J/mol×K	1097.80	Joback Method
cpg	951.06	J/mol×K	1144.33	Joback Method
cpg	974.05	J/mol×K	1190.87	Joback Method
cpg	999.18	J/mol×K	1237.40	Joback Method
cpg	1026.90	J/mol×K	1283.94	Joback Method
cpg	1057.66	J/mol×K	1330.47	Joback Method

dvisc	0.0046199	Paxs	713.08	Joback Method
dvisc	0.0041148	Paxs	769.44	Joback Method
dvisc	0.0037234	Paxs	825.81	Joback Method
dvisc	0.0034125	Paxs	882.17	Joback Method
dvisc	0.0031604	Paxs	938.53	Joback Method
dvisc	0.0029526	Paxs	994.90	Joback Method
dvisc	0.0027786	Paxs	1051.26	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C222753&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
dvisc:	Dynamic viscosity
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
ie:	Ionization energy
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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