Heptacene

Inchi: InChI=1S/C30H18/c1-2-6-20-10-24-14-28-18-30-16-26-12-22-8-4-3-7-21(22)11-25(26)15
InchiKey: KDEZIUOWTXJEJK-UHFFFAOYSA-N
Formula: C30H18
SMILES: c1ccc2cc3cc4cc5cc6cc7ccccc7cc6cc5cc4cc3cc2c1
Mol. weight [g/mol]: 378.46
CAS: 258-38-8

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
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	m3/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	Pa×s	713.08	Joback Method
dvisc	0.0041148	Pa×s	769.44	Joback Method

dvisc	0.0037234	Pa×s	825.81	Joback Method
dvisc	0.0034125	Pa×s	882.17	Joback Method
dvisc	0.0031604	Pa×s	938.53	Joback Method
dvisc	0.0029526	Pa×s	994.90	Joback Method
dvisc	0.0027786	Pa×s	1051.26	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C258388&Units=SI

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
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