

Naphtho[2,1,8-uva]pentaphene

Inchi:	InChI=1S/C28H16/c1-2-5-20-16-25-21(14-19(20)4-1)9-11-22-15-23-10-8-17-6-3-7-18-12
InchiKey:	DQYABORHGPGET-UHFFFAOYSA-N
Formula:	C28H16
SMILES:	c1ccc2cc3c(ccc4cc5ccc6cccc7ccc(c43)c5c67)cc2c1
Mol. weight [g/mol]:	352.43
CAS:	121159-18-0

Physical Properties

Property code	Value	Unit	Source
gf	883.28	kJ/mol	Joback Method
hf	658.89	kJ/mol	Joback Method
hfus	45.46	kJ/mol	Joback Method
hvap	92.71	kJ/mol	Joback Method
log10ws	-11.71		Crippen Method
logp	8.044		Crippen Method
mcvol	269.160	ml/mol	McGowan Method
pc	1947.51	kPa	Joback Method
tb	997.80	K	Joback Method
tc	1271.87	K	Joback Method
tf	696.82	K	Joback Method
vc	1.058	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	812.33	J/mol×K	997.80	Joback Method
cpg	830.69	J/mol×K	1043.48	Joback Method
cpg	850.20	J/mol×K	1089.16	Joback Method
cpg	871.30	J/mol×K	1134.83	Joback Method
cpg	894.41	J/mol×K	1180.51	Joback Method
cpg	919.98	J/mol×K	1226.19	Joback Method
cpg	948.44	J/mol×K	1271.87	Joback Method
dvisc	0.0086256	Pa×s	696.82	Joback Method
dvisc	0.0081349	Pa×s	746.98	Joback Method

dvisc	0.0077289	Pa×s	797.15	Joback Method
dvisc	0.0073878	Pa×s	847.31	Joback Method
dvisc	0.0070975	Pa×s	897.47	Joback Method
dvisc	0.0068476	Pa×s	947.64	Joback Method
dvisc	0.0066304	Pa×s	997.80	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=C121159180&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

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