sec-hexadecylnaphthalene

Inchi: InChI=1S/C26H40/c1-3-4-5-6-7-8-9-10-11-12-13-14-18-23(2)25-22-17-20-24-19-15-16-21
InchiKey: YRKSLYAWOBZISP-UHFFFAOYSA-N
Formula: C26H40
SMILES: CCCCCCCCCCCCCCC(C)c1cccc2ccccc12
Mol. weight [g/mol]: 352.60
CAS: 94247-63-9

Physical Properties

Property code	Value	Unit	Source
gf	375.03	kJ/mol	Joback Method
hf	-169.12	kJ/mol	Joback Method
hfus	50.24	kJ/mol	Joback Method
hvap	77.66	kJ/mol	Joback Method
log10ws	-9.90		Crippen Method
logp	9.035		Crippen Method
mcvol	333.980	ml/mol	McGowan Method
pc	1011.02	kPa	Joback Method
tb	844.48	K	Joback Method
tc	1044.68	K	Joback Method
tf	439.42	K	Joback Method
vc	1.300	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1063.18	J/mol×K	844.48	Joback Method
cpg	1083.45	J/mol×K	877.85	Joback Method
cpg	1102.61	J/mol×K	911.21	Joback Method
cpg	1120.76	J/mol×K	944.58	Joback Method
cpg	1137.98	J/mol×K	977.95	Joback Method
cpg	1154.34	J/mol×K	1011.32	Joback Method
cpg	1169.94	J/mol×K	1044.68	Joback Method
dvisc	0.0012229	Pa×s	439.42	Joback Method
dvisc	0.0005766	Pa×s	506.93	Joback Method

dvisc	0.0003244	Pa×s	574.44	Joback Method
dvisc	0.0002060	Pa×s	641.95	Joback Method
dvisc	0.0001426	Pa×s	709.46	Joback Method
dvisc	0.0001052	Pa×s	776.97	Joback Method
dvisc	0.0000815	Pa×s	844.48	Joback Method

Sources

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=C94247639&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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