1Hbenz[de]anthracene, hexadecahydro-6-octyl-

Other names: 6-n-Octyl-(hexadecahydrobenz(de)anthracene
6-n-Octylperhydrobenz(de)anthracene
6-Octyl(hexylhydrobenz[de]anthracene)
Inchi: InChI=1S/C25H44/c1-2-3-4-5-6-7-11-19-16-17-20-13-10-15-23-22-14-9-8-12-21(22)18-24
InchiKey: HOLRQJVOISUULR-UHFFFAOYSA-N
Formula: C25H44
SMILES: CCCCCCCCC1CCC2CCCC3C4CCCCC4CC1C23
Mol. weight [g/mol]: 344.62
CAS: 7225-65-2

Physical Properties

Property code	Value	Unit	Source
gf	318.99	kJ/mol	Joback Method
hf	-359.95	kJ/mol	Joback Method
hfus	45.76	kJ/mol	Joback Method
hvap	70.83	kJ/mol	Joback Method
log10ws	-8.17		Crippen Method
logp	8.006		Crippen Method
mcvol	319.670	ml/mol	McGowan Method
pc	1059.64	kPa	Joback Method
tb	805.70	K	Joback Method
tc	1014.61	K	Joback Method
tf	412.95	K	Joback Method
vc	1.220	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1125.98	J/mol×K	805.70	Joback Method
cpg	1152.94	J/mol×K	840.52	Joback Method
cpg	1178.24	J/mol×K	875.34	Joback Method
cpg	1201.99	J/mol×K	910.16	Joback Method
cpg	1224.31	J/mol×K	944.98	Joback Method
cpg	1245.30	J/mol×K	979.79	Joback Method

cpg	1265.09	J/mol×K	1014.61	Joback Method
dvisc	0.0042753	Pa×s	412.95	Joback Method
dvisc	0.0031469	Pa×s	478.41	Joback Method
dvisc	0.0024936	Pa×s	543.87	Joback Method
dvisc	0.0020773	Pa×s	609.33	Joback Method
dvisc	0.0017929	Pa×s	674.78	Joback Method
dvisc	0.0015882	Pa×s	740.24	Joback Method
dvisc	0.0014349	Pa×s	805.70	Joback Method
hvapt	93.80	kJ/mol	500.50	NIST Webbook

Sources

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=C7225652&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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
hvapt: Enthalpy of vaporization at a given temperature
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