

Octane, 3,6-diphenyl-

Inchi:	InChI=1S/C20H26/c1-3-17(19-11-7-5-8-12-19)15-16-18(4-2)20-13-9-6-10-14-20/h5-14,17
InchiKey:	DYCDLRHYBKZTGO-UHFFFAOYSA-N
Formula:	C20H26
SMILES:	CCC(CCC(CC)c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	266.42
CAS:	21411-33-6

Physical Properties

Property code	Value	Unit	Source
gf	337.46	kJ/mol	Joback Method
hf	6.37	kJ/mol	Joback Method
hfus	28.59	kJ/mol	Joback Method
hvap	63.89	kJ/mol	Joback Method
log10ws	-6.33		Crippen Method
logp	6.154		Crippen Method
mcvol	245.140	ml/mol	McGowan Method
pc	1652.46	kPa	Joback Method
tb	709.48	K	Joback Method
tc	931.76	K	Joback Method
tf	338.00	K	Joback Method
vc	0.927	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	689.23	J/molxK	709.48	Joback Method
cpg	777.57	J/molxK	894.71	Joback Method
cpg	762.38	J/molxK	857.67	Joback Method
cpg	746.04	J/molxK	820.62	Joback Method
cpg	728.45	J/molxK	783.57	Joback Method
cpg	709.55	J/molxK	746.53	Joback Method
cpg	791.69	J/molxK	931.76	Joback Method
dvisc	0.0000844	Paxs	709.48	Joback Method
dvisc	0.0001156	Paxs	647.57	Joback Method

dvisc	0.0001693	Paxs	585.65	Joback Method
dvisc	0.0002713	Paxs	523.74	Joback Method
dvisc	0.0004933	Paxs	461.83	Joback Method
dvisc	0.0010794	Paxs	399.91	Joback Method
dvisc	0.0031470	Paxs	338.00	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C21411336&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

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
mccvol:	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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