

Naphthalene, 1,4-dimethyl-5-octyl-

Other names:	1,4-Dimethyl-5-octylnaphthalene
Inchi:	InChI=1S/C20H28/c1-4-5-6-7-8-9-11-18-12-10-13-19-16(2)14-15-17(3)20(18)19/h10,12-
InchiKey:	BSKSLVGHMZRDL-UHFFFAOYSA-N
Formula:	C20H28
SMILES:	CCCCCCCCc1cccc2c(C)ccc(C)c12
Mol. weight [g/mol]:	268.44
CAS:	55000-53-8

Physical Properties

Property code	Value	Unit	Source
gf	307.69	kJ/mol	Joback Method
hf	-62.94	kJ/mol	Joback Method
hfus	37.45	kJ/mol	Joback Method
hvap	66.02	kJ/mol	Joback Method
log10ws	-7.54		Crippen Method
logp	6.360		Crippen Method
mcvol	249.440	ml/mol	McGowan Method
pc	1471.36	kPa	Joback Method
tb	717.60	K	Joback Method
tc	921.62	K	Joback Method
tf	411.84	K	Joback Method
vc	0.970	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	803.06	J/molxK	921.62	Joback Method
cpg	789.03	J/molxK	887.62	Joback Method
cpg	774.21	J/molxK	853.62	Joback Method
cpg	758.53	J/molxK	819.61	Joback Method
cpg	741.94	J/molxK	785.61	Joback Method
cpg	724.38	J/molxK	751.60	Joback Method
cpg	705.79	J/molxK	717.60	Joback Method
dvisc	0.0011164	Paxs	411.84	Joback Method

dvisc	0.0001778	Paxs	717.60	Joback Method
dvisc	0.0002148	Paxs	666.64	Joback Method
dvisc	0.0002678	Paxs	615.68	Joback Method
dvisc	0.0003474	Paxs	564.72	Joback Method
dvisc	0.0004746	Paxs	513.76	Joback Method
dvisc	0.0006944	Paxs	462.80	Joback Method
hvapt	81.60	kJ/mol	464.00	NIST Webbook

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55000538&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
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

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