Naphthalene, decahydro-1,1,4a-trimethyl-6-methylene-5-(3-meth [4aS-(4a«alpha»,5«alpha»,8a«beta»)]-

Other names:	Labda-8(20),13(16),14-triene
	Sclaren
	Sclarene
Inchi:	InChI=1S/C20H32/c1-7-15(2)9-11-17-16(3)10-12-18-19(4,5)13-8-14-20(17,18)6/h7,17-18
InchiKey:	KYLKKZSVPLUGCC-IKCNDWCXSA-N
Formula:	C20H32
SMILES:	C=CC(=C)CCC1C(=C)CCC2C(C)(C)CCCC12C
Mol. weight [g/mol]:	272.47
CAS:	511-02-4

Physical Properties

Property code	Value	Unit	Source
gf	384.43	kJ/mol	Joback Method
hf	-20.06	kJ/mol	Joback Method
hfus	19.94	kJ/mol	Joback Method
hvap	56.61	kJ/mol	Joback Method
log10ws	-6.58		Crippen Method
logp	6.308		Crippen Method
mcvol	258.040	ml/mol	McGowan Method
pc	1428.30	kPa	Joback Method
rinpol	1935.00		NIST Webbook
rinpol	1942.00		NIST Webbook
rinpol	1964.00		NIST Webbook
rinpol	1933.00		NIST Webbook
rinpol	1931.00		NIST Webbook
ripol	2233.00		NIST Webbook
ripol	2259.00		NIST Webbook
tb	671.10	K	Joback Method
tc	887.82	K	Joback Method
tf	372.48	K	Joback Method
vc	0.979	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	751.01	J/mol×K	671.10	Joback Method
cpg	775.70	J/mol×K	707.22	Joback Method
cpg	799.30	J/mol×K	743.34	Joback Method
cpg	822.04	J/mol×K	779.46	Joback Method
cpg	844.17	J/mol×K	815.58	Joback Method
cpg	865.92	J/mol×K	851.70	Joback Method
cpg	887.55	J/mol×K	887.82	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=C511024&Units=SI

Legend

cpg: Ideal gas heat capacity
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
rinpol: Non-polar retention indices
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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