

Kaurene

Inchi: InChI=1S/C20H32/c1-14-12-20-11-8-16-18(2,3)9-5-10-19(16,4)17(20)7-6-15(14)13-20/h1-20
InchiKey: ONVABDHFQKWOSV-GTSVPISWSA-N
Formula: C20H32
SMILES: C=C1CC23CCC4C(C)(C)CCCC4(C)C2CCC1C3
Mol. weight [g/mol]: 272.47
CAS: 34424-57-2

Physical Properties

Property code	Value	Unit	Source
gf	333.31	kJ/mol	Joback Method
hf	-100.29	kJ/mol	Joback Method
hfus	13.79	kJ/mol	Joback Method
hvap	56.54	kJ/mol	Joback Method
log10ws	-6.18		Crippen Method
logp	5.975		Crippen Method
mcvol	244.920	ml/mol	McGowan Method
pc	1693.51	kPa	Joback Method
rinpol	2043.00		NIST Webbook
rinpol	2034.00		NIST Webbook
rinpol	2019.00		NIST Webbook
rinpol	2043.00		NIST Webbook
rinpol	2034.00		NIST Webbook
rinpol	2041.00		NIST Webbook
rinpol	2043.00		NIST Webbook
rinpol	2043.00		NIST Webbook
rinpol	2036.00		NIST Webbook
rinpol	2034.00		NIST Webbook
rinpol	2034.00		NIST Webbook
rinpol	2045.00		NIST Webbook
rinpol	2043.00		NIST Webbook
rinpol	2034.00		NIST Webbook
rinpol	2008.00		NIST Webbook
rinpol	2038.00		NIST Webbook
rinpol	2071.00		NIST Webbook
rinpol	2036.00		NIST Webbook
rinpol	2012.00		NIST Webbook
rinpol	2048.00		NIST Webbook

rinpol	2027.00		NIST Webbook
rinpol	2034.00		NIST Webbook
rinpol	2025.00		NIST Webbook
rinpol	2014.00		NIST Webbook
rinpol	2023.00		NIST Webbook
rinpol	2025.00		NIST Webbook
rinpol	2025.00		NIST Webbook
rinpol	2043.00		NIST Webbook
rinpol	2036.00		NIST Webbook
ripol	2350.00		NIST Webbook
ripol	2350.00		NIST Webbook
ripol	2351.00		NIST Webbook
ripol	2425.00		NIST Webbook
ripol	2399.00		NIST Webbook
ripol	2393.00		NIST Webbook
tb	691.58	K	Joback Method
tc	933.36	K	Joback Method
tf	449.74	K	Joback Method
vc	0.927	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	768.47	J/mol×K	691.58	Joback Method
cpg	795.89	J/mol×K	731.88	Joback Method
cpg	822.42	J/mol×K	772.17	Joback Method
cpg	848.59	J/mol×K	812.47	Joback Method
cpg	874.91	J/mol×K	852.76	Joback Method
cpg	901.90	J/mol×K	893.06	Joback Method
cpg	930.06	J/mol×K	933.36	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=C34424572&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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