

(E)-3-Methyl-5-((1R,4aR,8aR)-5,5,8a-trimethyl-2-methyl-2-oxocyclohexane-1-carboxylic acid

Other names:
acid

Copalic acid

(-)-Copalic acid

Inchi: InChI=1S/C20H32O2/c1-14(13-18(21)22)7-9-16-15(2)8-10-17-19(3,4)11-6-12-20(16,17)5

InchiKey: JFQBNOIJWROZGE-VBRACAIISA-N

Formula: C20H32O2

SMILES: C=C1CCC2C(C)(C)CCCC2(C)C1CCC(C)=CC(=O)O

Mol. weight [g/mol]: 304.47

CAS: 20257-75-4

Physical Properties

Property code	Value	Unit	Source
gf	23.23	kJ/mol	Joback Method
hf	-418.51	kJ/mol	Joback Method
hfus	28.39	kJ/mol	Joback Method
hvap	81.33	kJ/mol	Joback Method
log10ws	-5.82		Crippen Method
logp	5.596		Crippen Method
mvol	269.780	ml/mol	McGowan Method
pc	1570.96	kPa	Joback Method
rinpol	2380.00		NIST Webbook
rinpol	2380.00		NIST Webbook
tb	827.95	K	Joback Method
tc	1039.75	K	Joback Method
tf	481.67	K	Joback Method
vc	1.022	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	884.27	J/molxK	827.95	Joback Method
cpg	905.84	J/molxK	863.25	Joback Method
cpg	927.32	J/molxK	898.55	Joback Method
cpg	948.95	J/molxK	933.85	Joback Method
cpg	970.94	J/molxK	969.15	Joback Method

cpg	993.53	J/mol×K	1004.45	Joback Method
cpg	1016.94	J/mol×K	1039.75	Joback Method

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=C20257754&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
hvac:	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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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