1-Naphthalenecarboxylic acid, decahydro-1,4a-dimethyl-6-methylene-5-(3-methyl ester, [1S-[1«alpha»,4a«alpha»,5«alpha»(E),8a«beta»]]-

Other names: Labda-8(20),12,14-trien-19-oic acid, methyl ester, (E)-
Methyl communate
Methyl trans-communate
Methyl 8(17), E-12,14-labdatrien-19-oate
Methyl ester of trans-communic acid
(E)-Methyl communate

Inchi: InChI=1S/C21H32O2/c1-7-15(2)9-11-17-16(3)10-12-18-20(17,4)13-8-14-21(18,5)19(22)2

InchiKey: WYJKGKPQXWDIQP-OQLLNIDSSA-N

Formula: C21H32O2

SMILES: C=CC(C)=CCC1C(=C)CCC2C(C)(C(=O)OC)CCCC12C

Mol. weight [g/mol]: 316.48

CAS: 15798-13-7

Physical Properties

Property code	Value	Unit	Source
gf	151.31	kJ/mol	Joback Method
hf	-293.71	kJ/mol	Joback Method
hfus	26.80	kJ/mol	Joback Method
hvap	68.62	kJ/mol	Joback Method
log10ws	-5.86		Crippen Method
logp	5.461		Crippen Method
mcvol	279.570	ml/mol	McGowan Method
pc	1386.08	kPa	Joback Method
rinpol	2234.00		NIST Webbook
rinpol	2256.00		NIST Webbook
rinpol	2256.00		NIST Webbook
tb	777.75	K	Joback Method
tc	998.78	K	Joback Method
tf	452.59	K	Joback Method
vc	1.058	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	874.20	J/mol×K	777.75	Joback Method
cpg	897.71	J/mol×K	814.59	Joback Method
cpg	920.73	J/mol×K	851.43	Joback Method
cpg	943.49	J/mol×K	888.26	Joback Method
cpg	966.25	J/mol×K	925.10	Joback Method
cpg	989.25	J/mol×K	961.94	Joback Method
cpg	1012.76	J/mol×K	998.78	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C15798137&Units=SI
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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume