1-Naphthalenepentanoic acid, 1,4,4a,5,6,7,8,8a-octahydro-«beta»,2,5,5,8a-pentar

Other names: Labd-7-en-15-oic acid
Catavic acid
Cativic acid

Inchi: InChI=1S/C20H34O2/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: FEENGIUGOPKQTF-UHFFFAOYSA-N

Formula: C20H34O2

SMILES: CC1=CCC2C(C)(C)CCCC2(C)C1CCC(C)CC(=O)O

Mol. weight [g/mol]: 306.48

CAS: 468-82-6

Physical Properties

Property code	Value	Unit	Source
gf	-83.63	kJ/mol	Joback Method
hf	-569.15	kJ/mol	Joback Method
hfus	27.97	kJ/mol	Joback Method
hvap	81.70	kJ/mol	Joback Method
log10ws	-5.73		Crippen Method
logp	5.676		Crippen Method
mcvol	274.080	ml/mol	McGowan Method
pc	1514.03	kPa	Joback Method
rinpol	2334.70		NIST Webbook
rinpol	2334.70		NIST Webbook
tb	828.45	K	Joback Method
tc	1036.19	K	Joback Method
tf	485.31	K	Joback Method
vc	1.036	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	911.37	J/mol×K	828.45	Joback Method
cpg	933.16	J/mol×K	863.07	Joback Method
cpg	954.78	J/mol×K	897.70	Joback Method
cpg	976.42	J/mol×K	932.32	Joback Method

cpg	998.30	J/mol×K	966.94	Joback Method
cpg	1020.63	J/mol×K	1001.57	Joback Method
cpg	1043.60	J/mol×K	1036.19	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C468826&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