Labd-8-en-15-ol

Inchi: InChI=1S/C20H36O/c1-15(11-14-21)7-9-17-16(2)8-10-18-19(3,4)12-6-13-20(17,18)5/h15
InchiKey: XKPWXFGNKDNUCP-JSFUQZLZSA-N
Formula: C20H36O
SMILES: CC1=C(CCC(C)CCO)C2(C)CCCC(C)(C)C2CC1
Mol. weight [g/mol]: 292.50

Physical Properties

Property code	Value	Unit	Source
gf	43.37	kJ/mol	Joback Method
hf	-447.70	kJ/mol	Joback Method
hfus	24.91	kJ/mol	Joback Method
hvap	75.92	kJ/mol	Joback Method
log10ws	-6.13		Crippen Method
logp	5.728		Crippen Method
mcvol	272.510	ml/mol	McGowan Method
pc	1462.37	kPa	Joback Method
rinpol	2216.00		NIST Webbook
tb	784.23	K	Joback Method
tc	986.10	K	Joback Method
tf	452.14	K	Joback Method
vc	1.032	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	881.66	J/mol×K	784.23	Joback Method
cpg	903.59	J/mol×K	817.87	Joback Method
cpg	925.16	J/mol×K	851.52	Joback Method
cpg	946.56	J/mol×K	885.16	Joback Method
cpg	967.98	J/mol×K	918.81	Joback Method
cpg	989.60	J/mol×K	952.45	Joback Method
cpg	1011.62	J/mol×K	986.10	Joback Method

Sources

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=R229222&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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