

labd-7,13-(E)-dien-15-ol

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C20H34O/c1-15(11-14-21)7-9-17-16(2)8-10-18-19(3,4)12-6-13-20(17,18)5/h8,11,13,15,17,19-20,21/t12,14,16,18,20

KPOGKOXAZMFZNM-ATJFKVBJSA-N

C20H34O

CC(=CCO)CCC1C(C)=CCC2C(C)(C)CCCC12C

290.48

Physical Properties

Property code	Value	Unit	Source
gf	119.40	kJ/mol	Joback Method
hf	-343.86	kJ/mol	Joback Method
hfus	28.79	kJ/mol	Joback Method
hvap	75.38	kJ/mol	Joback Method
log10ws	-5.99		Crippen Method
logp	5.504		Crippen Method
mcvol	268.210	ml/mol	McGowan Method
pc	1497.67	kPa	Joback Method
rinpol	2280.00		NIST Webbook
rinpol	2280.00		NIST Webbook
ripol	2507.00		NIST Webbook
ripol	2507.00		NIST Webbook
tb	779.06	K	Joback Method
tc	985.17	K	Joback Method
tf	431.34	K	Joback Method
vc	1.018	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	858.87	J/mol×K	779.06	Joback Method
cpg	880.81	J/mol×K	813.41	Joback Method
cpg	902.39	J/mol×K	847.76	Joback Method
cpg	923.82	J/mol×K	882.11	Joback Method
cpg	945.31	J/mol×K	916.47	Joback Method
cpg	967.09	J/mol×K	950.82	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=R327683&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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