

Betunal

Inchi:	InChI=1S/C30H48O2/c1-19(2)20-10-15-30(18-31)17-16-28(6)21(25(20)30)8-9-23-27(5)1
InchiKey:	FELCJAPFJOPHSD-UHFFFAOYSA-N
Formula:	C30H48O2
SMILES:	C=C(C)C1CCC2(C=O)CCC3(C)C(CCC4C5(C)CCC(O)C(C)(C)C5CCC43C)C12
Mol. weight [g/mol]:	440.70
CAS:	13159-28-9

Physical Properties

Property code	Value	Unit	Source
gf	202.11	kJ/mol	Joback Method
hf	-503.50	kJ/mol	Joback Method
hfus	30.25	kJ/mol	Joback Method
hvap	98.17	kJ/mol	Joback Method
log10ws	-7.95		Crippen Method
logp	7.204		Crippen Method
mcvol	382.400	ml/mol	McGowan Method
pc	1069.36	kPa	Joback Method
rinpol	3628.60		NIST Webbook
rinpol	3628.60		NIST Webbook
tb	1055.70	K	Joback Method
tc	1299.98	K	Joback Method
tf	677.60	K	Joback Method
vc	1.454	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1607.54	J/mol×K	1055.70	Joback Method
cpg	1667.51	J/mol×K	1096.41	Joback Method
cpg	1733.47	J/mol×K	1137.13	Joback Method
cpg	1806.22	J/mol×K	1177.84	Joback Method
cpg	1886.57	J/mol×K	1218.56	Joback Method
cpg	1975.34	J/mol×K	1259.27	Joback Method
cpg	2073.36	J/mol×K	1299.98	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13159289&Units=SI
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

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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