

D:A-Friedooleanan-3-ol, (3«alpha»)-

Other names:	D:A-Friedooleanan-3«alpha»-ol Friedelan-3«alpha»-ol Friedelanol Friedelinol Friedelan-3-ol
Inchi:	InChI=1S/C30H52O/c1-20-21(31)9-10-22-27(20,5)12-11-23-28(22,6)16-18-30(8)24-19-2
InchiKey:	XCDQFROEGGNAER-UHFFFAOYSA-N
Formula:	C30H52O
SMILES:	CC1C(O)CCC2C1(C)CCC1C2(C)CCC2(C)C3CC(C)(C)CCC3(C)CCC12C
Mol. weight [g/mol]:	428.73
CAS:	5085-72-3

Physical Properties

Property code	Value	Unit	Source
gf	204.75	kJ/mol	Joback Method
hf	-524.48	kJ/mol	Joback Method
hfus	22.16	kJ/mol	Joback Method
hvap	91.06	kJ/mol	Joback Method
log10ws	-8.81		Crippen Method
logp	8.249		Crippen Method
mcvol	385.130	ml/mol	McGowan Method
pc	1034.57	kPa	Joback Method
rinpol	3123.00		NIST Webbook
rinpol	3123.00		NIST Webbook
tb	1014.99	K	Joback Method
tc	1257.85	K	Joback Method
tf	671.70	K	Joback Method
vc	1.446	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1602.08	J/mol×K	1014.99	Joback Method
cpg	1663.28	J/mol×K	1055.47	Joback Method

cpg	1730.65	J/mol×K	1095.94	Joback Method
cpg	1805.09	J/mol×K	1136.42	Joback Method
cpg	1887.50	J/mol×K	1176.90	Joback Method
cpg	1978.78	J/mol×K	1217.37	Joback Method
cpg	2079.83	J/mol×K	1257.85	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=C5085723&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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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