Friedelan-3-one

Other names:	Friedelin
	D:A-Friedooleanan-3-one
	Friedeline
	Friedlein
	(4R,4aS,6aS,6bR,8aR,12aR,12bS,14aS,14bS)-4,4a,6b,8a,11,11,12b,14a-Octamethylicos
Inchi:	InChI=1S/C30H50O/c1-20-21(31)9-10-22-27(20,5)12-11-23-28(22,6)16-18-30(8)24-19-25
InchiKey:	OFMXGFHWLZPCFL-UHFFFAOYSA-N
Formula:	C30H50O
SMILES:	CC1C(=O)CCC2C1(C)CCC1C2(C)CCC2(C)C3CC(C)(C)CCC3(C)CCC12C
Mol. weight [g/mol]:	426.72
CAS:	559-74-0

Physical Properties

Property code	Value	Unit	Source
gf	226.69	kJ/mol	Joback Method
hf	-489.61	kJ/mol	Joback Method
hfus	16.51	kJ/mol	Joback Method
hvap	78.94	kJ/mol	Joback Method
log10ws	-8.72		Crippen Method
logp	8.457		Crippen Method
mcvol	380.830	ml/mol	McGowan Method
pc	1018.78	kPa	Joback Method
rinpol	2858.00		NIST Webbook
rinpol	3510.60		NIST Webbook
rinpol	2858.00		NIST Webbook
rinpol	2858.00		NIST Webbook
rinpol	3510.60		NIST Webbook
tb	995.30	K	Joback Method
tc	1256.59	K	Joback Method
tf	683.34	K	Joback Method
vc	1.435	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1548.17	J/mol×K	995.30	Joback Method
cpg	1610.31	J/mol×K	1038.85	Joback Method
cpg	1678.89	J/mol×K	1082.40	Joback Method
cpg	1754.96	J/mol×K	1125.95	Joback Method
cpg	1839.61	J/mol×K	1169.49	Joback Method
cpg	1933.91	J/mol×K	1213.04	Joback Method
cpg	2038.93	J/mol×K	1256.59	Joback Method

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C559740&Units=SI

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

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