Naphtho[2,1-b]furan, dodecahydro-3a,6,6,9a-tetramethyl (Amberlyn)

Inchi: InChI=1S/C16H28O/c1-11-5-8-15(2,3)12-6-9-16(4)13(14(11)12)7-10-17-16/h11-14H,5-10

InchiKey: IRMZQMQKCHSNKX-UHFFFAOYSA-N

Formula: C16H28O

SMILES: CC1CCC(C)(C)C2CCC3(C)OCCC3C12

Mol. weight [g/mol]: 236.39

Physical Properties

Property code	Value	Unit	Source
gf	97.46	kJ/mol	Joback Method
hf	-342.35	kJ/mol	Joback Method
hfus	21.80	kJ/mol	Joback Method
hvap	52.92	kJ/mol	Joback Method
log10ws	-4.19		Crippen Method
logp	4.264		Crippen Method
mcvol	209.590	ml/mol	McGowan Method
pc	1920.30	kPa	Joback Method
rinpol	1767.00		NIST Webbook
rinpol	1767.00		NIST Webbook
tb	616.20	K	Joback Method
tc	847.19	K	Joback Method
tf	371.47	K	Joback Method
vc	0.784	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	618.87	J/mol×K	616.20	Joback Method
cpg	644.95	J/mol×K	654.70	Joback Method
cpg	669.49	J/mol×K	693.20	Joback Method
cpg	692.80	J/mol×K	731.70	Joback Method
cpg	715.16	J/mol×K	770.19	Joback Method
cpg	736.87	J/mol×K	808.69	Joback Method
cpg	758.22	J/mol×K	847.19	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=R576642&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